Supplementary Information

Anisotropic Kinetics of Solid Phase Transition from First Principles: Alpha-Omega Phase Transformation of Zr

Shu-Hui Guan, Zhi-Pan Liu*

Collaborative Innovation Center of Chemistry for Energy Material, Key Laboratory of Computational Physical Science (Ministry of Education), Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Department of Chemistry, Fudan University, Shanghai 200433, China

- Part 1. The α-ω crystallographic orientation relationships in literatures
- Part 2. Theoretical methods
 - a. Stochastic Surface Walking (SSW) pathway sampling
 - b. DFT calculation
 - c. Phonon and elastic property
- Part 3. Pressure dependence of homogeneous phase transition pathways (P-I and P-II)
- Part 4. Numerical search to determine the OR and search for atomic habit planes (coherent interface)
- Part 5. Heterophase junctions in superlattice (HJ-I to HJ-VI in Table 1)
- Part 6. The Cartesian atomic coordinates for P-I, P-II, P(HJ-I) and P(HJ-II)

Part 1. The α - ω crystallographic orientation relationships in literatures

	Conditions	Variant-I OR	Variant-II OR
J. M. Silcock[1]	TiV, TiMo and TiCr alloys;		$(0001)\alpha (11\bar{2}0)\omega;$
(Silcock) 1958	XRD		$[1\bar{2}0]\alpha \ [0001]\omega$ (Silcock
			OR = UZ Variant-II OR)
M. P. Usikov and V. A. Zilbershtei ¹	Zr, Ti under static pressure (10	$(0001)\alpha//(01\overline{1}1)\omega;$ [11 $\overline{2}0$] $\alpha//[10\overline{1}1]\omega$	(0001)α//(11 <u>2</u> 0)ω;
(UZ) 1973	GPa); Theory and TEM	(observed in	[1120]α//[0001]ω
		experiment)	(not observed in experiment)
A. Rabinkin, M. Talianker and O. Botstein ² (RTB) 1980	Zr under static pressure (6 GPa); high resolution dark-field electron microscopy and selected area diffraction(SAD)		(0001)α//(1210)ω; [2110]α//[0001]ω variant1 (0001)α//(1210)ω; [1120]α//[0001]ω variant2 (0001)α//(1210)ω; [1210]α//[0001]ω variant3 (RTB OR=UZ Variant-II OR)
Kutsar et al ³ 1990	Shock samples Zr (8-32 GPa)		(0001)α//(1120)ω;
	Reverse $\omega \rightarrow \alpha$; XRD, TEM		$[\overline{1}\overline{1}20]\alpha/[0001]\omega$
S. Song and G. T. Gray ⁴ (SG) 1995	Zr shock-loaded (7 GPa); SAD,TEM	$(0001)\alpha //(10\bar{1}1)\omega;$ $[10\bar{1}0]\alpha //[11\bar{2}\bar{3}]\omega$ (SG = UZ Variant-I OR)	
G. Jyoti, K.D. Joshi , Satish C. Gupta,Sikka SK 1997 ⁵	Shock-loaded Zr (11.8GPa) SAD,TEM	UZ ORI, also SG	
D. R. Trinkle, R.G.	Ti	$(0001)\alpha//(0\overline{1}11)\omega;$ [1120] $\alpha//[01\overline{1}1]\omega;$	
J.W.Wilkins ⁶ 2003	Theory	(TAO-1= UZ Variant-I OR)	
G.T. Gray ⁷ 2005	Highest purity Zr under static pressure (7.1-8 GPa); SEM, TEM	$(0001)\alpha/(\bar{1}101)\omega;$ $[\bar{1}010]\alpha/[\bar{2}11\bar{3}]\omega$	
Jyoti G 2008 ⁸	Shock compressed Zr (11.6	Confirm UZ	

Table SI The orientat	ion relations (OR) for α - ω phase t	ransition in literatures	(not limited to Zr).

	GPa)	Variant-I OR	
	TEM, XRD, SAD		
Wenk Kaercher ⁹	Zr D-DIA and DAC at 1.5-4.5		$(0001)\alpha //(11\bar{2}0)\omega;$
2013	GPa; in situ synchrotron x-ray		[1120]α//[0001]ω; highly
	diffraction;		reversible
Zong, Lookman ¹⁰	Anisotropic shock response of	Shock along	Shock along $[10\overline{1}0]\alpha$ and
2014		[0001]α	[1210]α
	Ti using molecular dynamics	$(0001)\alpha/(10\overline{1}0)\omega;$	$(0001)\alpha //(11\bar{2}0)\omega;$
	(Theory)	[1010]α//[1123]ω	[1120]α//[0001]ω
Zong, Lookman ¹¹	Zr Ti 15-20 µm, shock at 8		$(0001)\alpha //(11\bar{2}0)\omega;$
2014	GPa recovered samples $\omega \rightarrow \alpha$		$[11\bar{2}0]\alpha / [0001]\omega$
	XRD		Reversibility,
			Heterogeneous nucleation
			observed

Part 2 Theoretical methods

a. Stochastic Surface Walking (SSW) pathway sampling

The SSW methodology has been described in our previous work in detail^{12, 13}. We have shown that the SSW method is able to explore the potential energy surface (PES) to identify unexpected new structures, including clusters and crystals, and at the mean time to collect the reaction pathways leading to them. This is attributed to the fact that SSW PES searching involves generally small displacement on lattice and atoms, and thus the pathway information is maintained from one minimum to another.

The purpose of SSW crystal pathway sampling is to establish a one-to-one correspondence for lattice $(L(e_1,e_2,e_3), e_i)$ being the lattice vector) and atom $(q_i, i=1,..3N, N)$ is the number of atom in cell) from one phase to another. The lattice here does not necessarily be the conventional Bravais lattice but any possible set of lattice that describe the same crystal phase. Using such a pair of coordinates, $Q_{IS}(L,q)$ and $Q_{FS}(L,q)$ (IS and FS are the initial and the final states), it is then possible to utilize double-ended transition state searching method to identify the reaction pathway and the transition state. The current approach is different from the traditional Landau-type theory where the lattice correspondence needs to be assumed. The procedure is described below briefly.

Pathway collection In SSW pathway sampling, firstly, we start from one single phase (starting phase), and utilize the SSW method to explore all the likely phases nearby the phase. A structure selection module is utilized to decide whether to accept/refuse once a new minimum is reached. If the new phase different from the starting phase is identified by the SSW crystal method¹⁴, we record/output the IS (i.e. starting phase) and the FS (a new phase) of the current SSW step. Then, the program will return back to the IS by rejecting the new minimum to continue the phase exploration; On the other hand, if the new minimum identified by SSW is still the starting phase (e.g. the same symmetry but a permutation isomer with varied lattice), the program will accept the new isomeric phase and start the phase exploration from this phase. We repeat this procedure until a certain number of IS/FS pairs are reached.

Pathway screening Secondly, we utilize the variable-cell double-ended surface walking (DESW) method¹⁵ to establish the pseudopathway connecting IS to FS for all IS/FS pairs ^{16, 17}. The approximate barrier is obtained according to DESW pseudopathway, where the maximum energy point along the pathway is generally a good estimate for the true TS ¹⁵. By sorting the approximate barrier height, we can obtain the candidates for lowest energy pathways.

It might be mentioned that at this stage, we generally examined thoroughly all the pathways we identified. Basically, even before we locate exactly the TS, we can have the following important information, including the approximate barrier, the pattern of lattice and atom movement from IS to FS, the atomic habit plane and the OR for the pathways, From these, we can safely rule out the similar pathways and focus on the selected, distinct and low energy pathways.

Lowest energy pathway determination Thirdly, the candidate lowest energy pathways are selected to locate exactly the "true" TS by using DESW TS-search method¹⁵. By sorting the exact barrier calculated, the energy difference between the TS and the IS, the lowest energy pathways can be finally obtained. All the lowest energy pathways will be further confirmed by extrapolating TS towards IS and FS, and the TSs are validated by phonon spectrum calculation, showing one and only one imaginary mode.

For α - ω phase transition in this work, starting either from α or ω phase, the DFT-based SSW pathway sampling in the 6-atom cell simulation visits 5777 minima nearby IS (see PES shown in Figure 2a) and collects 233 IS/FS pairs (see Figure S1 below); in the 12-atom cell simulation, visits 2193 minima and collects 33 IS/FS pairs. All the calculations were performed under 3 GPa hydrostatic pressure.

Figure S1 plots the structure of high-symmetry Zr crystal phases obtained from SSW sampling. We can identify all the common phases, including the simple hexagonal phase (ω , the global minimum at 3 GPa), the α phase, the body-center cubic (bcc, no. 229), and also other possible phases, such as face-center cubic (fcc, no.225) and a cubic phase (no.139). These phases can be distinguished by their symmetry, the volume and the coordination of Zr. In this work, the coordination is defined as Eq. S1 below

$$C = \frac{C_0}{N_0} \sum_{i=1}^{N_0} \sum_{j=1(i\neq j)}^{N} \frac{1}{1 + e^{d_{ij} - d_0}}$$
(S1)

where N_0 is the number of Zr atoms in the primitive cell and N is the number of Zr atoms in the supercell ((3x3x3) of the primitive cell), *i* and *j* are the label of atom; d_{ij} is the distance between the *i* atom and *j* atom; d_0 is a constant being 3.24 (Å); C₀ is a scaling constant being 1.33 to yield ~12-coordination for Zr in α phase.

Figure S1 plots the approximate barrier from DESW peudopathways against the scaled Euclidean distance of the pathway for α - ω phase transitions. It includes the results from both 6-atom and 12-atom sampling. In the 6-atom sampling, 51 of 233 pathways have the approximate barrier below 90 meV/atom with respect to α phase. Among them, 13 lowest energy pathways in the bottom left corner were selected for the exact TS location. This leads to the finding of the lowest energy pathways, **P-I to P-IV** (see Figure 1b and also Figure S1). In the 12-atom sampling, 16 of 37 pathways have the approximate barrier below 90 meV/atom with respect to α phase. Among them, 12 lowest energy pathways in the bottom left corner were selected for the exact TS location. This leads to the finding of the same lowest energy pathways, **P-I** and **P-II**.



Figure S1. Pathway screening by plotting the approximate energy barrier (eV/6-atom with respect to α phase) versus the scaled Euclidean distance (Å) between two phases (measured from the pathways) under 3 GPa. In

total, there are 233 pathways from 6-atom sampling and 37 pathways from 12-atom sampling. The approximate barrier is obtained according to DESW pseudopathway, where the maximum energy point along the pathway is generally a good estimate for the true TS¹⁵. Only the lowest energy pathways, **P-I** to **P-III** are highlighted.



Figure S2 Potential energy profile for five lowest energy pathways for α - ω solid phase transition, **P-I** to **P-V** (**P-I** to **P-III** are also discussed in the text).

b. DFT calculation details

All calculations were perfomed using the plane wave DFT program, Vienna ab initio simulation package VASP ^{18, 19} where Zr electron-ion interaction was represented by the projector augmented wave $(PAW)^{20}$ and the exchange-correlation functional utilized was GGA-PBE²¹. In the pathway sampling, we adopt the following setups to speed up the PES exploration: plane-wave cutoff 400 eV; the Monkhorst-Pack k-point mesh of (6×6×6) set for 6-atom supercell and (4×4×4) set for 12-atom supercell; 4-electron (4d5s5p) PAW pesudopotential for Zr. To obtain accurate energetics for the pathways, a more accurate calculation setup was utilized: the plane-wave cutoff 600 eV; the k-point mesh up to (10×10×10) set and 12-electron (4s4p4d5s5p) PAW pesudopotential for Zr. For all the structures, both lattice and atomic positions were fully optimized until the maximal stress component is below 0.1 GPa and the maximal force component below 0.001 eV/Å, which leads to the convergence of the relative energy (e.g. barrier) below 2 meV/atom. The convergence of the energetics with respect to k-point mesh is shown in Table SII.

TABLE SII The convergence of energetics (meV/atom) for the key states (6-atom cell, see Part 6 for structures) in P-II with respect to different k-point mesh. The energy of α -phase is set as zero reference. The TS has been re-optimized under each k-point set.

k -point mesh	6×4×6	8×6×8	8×8×8	10×8×10
α phase	0	0	0	0
TS2	51.58	53.67	53.27	51.62
ω phase	-2.31	-4.84	-4.94	-4.71

c. Phonon and elastic properties

The phonon frequencies of the crystals were determined using the finite displacement method^{22, 23}, employing the PHONOPY package ²⁴. In these calculations, the size of the system was increased to $(2 \times 2 \times 2)$ supercell (48-atom supercell) and the K-point utilized is $(2 \times 2 \times 2)$ Monkhorst-Pack mesh. With a displacement of ±0.01 Å on nonequivalent atoms, a set of displaced supercells was generated and the forces

of these supercells were calculated using plane-wave DFT package, VASP program. These forces were carried back to the PHONOPY to calculate the phonon dispersion curves. The TS phonon spectra are shown in Figure S4, confirming one and only one negative phonon mode in the Brillion zone for the TS obtained in this work.

The elastic tensor is determined by performing six finite distortions of the lattice and deriving the elastic constants from the strain-stress relationship²⁵. The linear elastic constants C_{ij} from a 6×6 symmetric matrix, have 27 different components, fulfilling $\sigma_i = C_{ij}\varepsilon_j$ for small stresses σ and strains ε values²⁶. Properties such as the bulk modulus, shear modulus can be computed from C_{ij} .

Specifically, the bulk modulus (B) and shear modulus (G) can be estimated from the individual elastic constants C_{ij} by the Voigt approximation and the Reuss approximation^{27, 28}. The expressions for the Voigt and Reuss approaches are represented in Eqs. (S2-3) for bulk and shear modulus:

$$B_{\nu} = \frac{1}{9}(C_{11} + C_{22} + C_{33}) + \frac{2}{9}(C_{12} + C_{23} + C_{13})$$
(S2)

$$G_{\nu} = \frac{1}{15}(C_{11} + C_{22} + C_{33}) - \frac{1}{15}(C_{12} + C_{23} + C_{13}) + \frac{1}{5}(C_{44} + C_{55} + C_{66}) \quad (S3)$$

Part 3. Pressure dependence of homogeneous phase transition pathways (P-I and P-II)

To understand the pressure dependence of the α - ω solid phase transition, we have also calculated the enthalpy barrier of the lowest energy homogeneous phase transition pathways, P-I and P-II, under different pressure conditions. The results are shown in Figure S3. We found that the barrier of P-I changes slightly with the change of the pressure, while the barrier of P-II decreases quite rapidly with the increase of the pressure. Nevertheless, the barrier of P-II is always higher than that of P-I at the interested pressure regions, even at the high pressures, e.g. 12 GPa. This indicates that P-I is always the preferred homogeneous phase transition channels that could be responsible for the initial nucleation events. Therefore, the observation on two different ORs in experiment cannot be attributed to the homogeneous phase transition mechanism alone. In the main text, we have shown in Figure 3 that it is the heterogeneous phase propagation pathways that are responsible for the pressure dependence of α - ω solid phase transition observed in experiment.



Figure S3. DFT enthalpy barrier with respect to α phase as a function of hydrostatic pressure for the homogeneous transition pathways P-I and P-II.

Part 4. Numerical search to determine the OR and search for atomic habit planes (coherent interface)



Figure S4. Snapshots for α - ω transformation in the homogeneous phase transition pathways, **P-I and P-II**. In the top panel are the views from $[0001]_{\omega}$ direction. Yellow lines are the atomic habit plane edge. The blue atoms highlights the atom row with zero displacement at $[0001]_{\omega}$ during the phase transition. Those in the bottom panel highlight the atom displacement viewed down from the determined atomic habit plane, $(11\overline{2}2)_{\alpha}$ (P-I) and $(10\overline{1}0)_{\alpha}$ (P-II). The distances labeled are in Å. Cyan and Grey: Zr at two different layers.

The SSW pathway sampling provides the lowest energy pathway between two connecting phases, which determines the lattice and atom correspondence, as illustrated in Figure S4 for α - ω phase transition in **P-I** and **P-II**. The lattice parameters and atomic coordinates of **P-II** utilized in the following analysis are provided in **Part 6**. Note that the lattice and atom coordinates identified in the lowest pathways are generally not in conventional Bravais lattice of crystal. In the following, we describe in detail the three steps that are required to identify the atomic habit plane (coherent interface) between two phases.

Step1: Determine Strain Invariant (minimum) Planes

Based on the lattice correspondence, we can first use the classical phenomenological theory of Martensitic crystallography (PTMC)²⁹⁻³⁵ to determine the invariant line strain, the possible habit planes and ORs.

Determine the principal axes of the phase transformation.

Let define two lattices as T and M, both (3x3) matrix of lattice.

A deformation gradient F matrix transform an initial lattice T to a final lattice M, as

FT= RBT=M

F=RB

where R is a rigid-body rotation matrix and B is a lattice deformation matrix, representing the generalized Bain deformation. In PTMC, **F** is also known as a homogeneous *invariant line strain*. The Gauchy-Green deformation tensor is

$$C = F^{T}F = (T^{T})^{-1} M^{T} MT^{-1}$$

C is rotational invariant.

The principal axes are the eigenvectors $(e_i, i=1,2,3)$ of the Gauchy-Green deformation tensor

The strain energy of the lattice deformation is defined the sum of three eigenvalues, \mathbf{l}_i

 $I = tr(\mathbf{F}^{\mathrm{T}}\mathbf{F}) = \mathbf{l}_{1} + \mathbf{l}_{2} + \mathbf{l}_{3}$

Taking **P-II** in α - ω phase transition as the example (which is simpler because its Martensitic mechanism), three principal axes (Cartesian coordinate) are as follows using α -phase as initial phase and ω -phase as final phase:

e₁: $(0.0084 \ 0.6913 \ -0.7225)_{\alpha}$; **l**₁=0.83077**e**₂: $(1.0000 \ -0.0049 \ 0.0070)_{\alpha}$; **l**₂=0.95218 **e3:** $(-0.0013 \quad 0.7226 \quad 0.6913)_{\alpha};$ **l3**= 1.23703

Obviously, e₂ direction is the principal axes with the lowest strain.

Determine the strain invariant lines (SIL) and strain invariant planes (SIP)

For Martensitic phase transition, three eigenvalues of matrix C could not be all larger than one or all smaller than 1 and in general l_2 should be close to unity for generating SIP (otherwise only strain minimum planes can be obtained):,

 $l_1 < 1; l_2 > 1; l_3 > 1;$ or $l_1 < 1; l_2 < 1; l_3 > 1$ $(l_3 > l_2 > l_1)$

Using three eigenvectors \mathbf{e} as the basis, we need to determine the strain invariant lines on a corn surrounding the maximum or the smallest \mathbf{e}_{i} . This is equivalent to find the fractional coordinate (a,b,c) in the following two equations.

$$a^{2}+b^{2}+c^{2}=1$$

 a^{2} $\mathbf{l}_{1}+b^{2}$ $\mathbf{l}_{2}+c^{2}$ $\mathbf{l}_{3}=1$

While there are in principle infinite number of solutions for (a,b,c), the problem can be simplified by identifying the strain invariant lines on the plane defined by the largest and the smallest eigenvectors, \mathbf{e}_1 and \mathbf{e}_3 ., i.e. by setting

b=0

These strain invariant lines can thus be solved as

 $sil_1 = ae_1 + ce_3$ and $sil_2 = ae_1 - ce_3$

In **P-II** of α - ω phase transition, two solutions of *sil* (Cartesian coordinate) vector on the plane with $\mathbf{e}_1 \times \mathbf{e}_3$ normal are yielded: sil₁: (0.0056 0.9944 $-0.1057)_{\alpha}$ $(-0.0073 - 0.0617 0.9981)_{a}$ sil₂: Similarly, the SILs on the plane defined by e_2 and e_3 can be found (in these cases, a nonzero strain on the principal axis e1 will be considered in the following step to generate strain minimum planes): sil₃: (0.9116 0.2916 $0.2896)_{a}$ sil₄: (-0.9127 0.3005 0.2768)

Using a *sil* vector and another untilted line, e.g. the principal axes **e** normal to *sil*, it is possible to construct the so-called strain invariant (minimum) plane, the habit plane. All lines on habit plane are unrotated, which should contain a strain invariant line and also an untilted line. These lines and their angle are unchanged under the rigid-body rotation and the lattice deformation. The habit plane normal *sip*, a unit vector, can be solved using

 $sip_k = sil_i \times e_j$ F $sip_k = RB sip_k = sip_k$

In **P-II** of α - ω phase transition, two solutions of *sip*_{*i*}, i=1, 2 with the minimum strain are yielded. In the convention of Miller plane, *sip* are named using (hkl) with real numbers:

sip₁: (0.0332)-0.8978 $-3.0609)_{g}$ $sip_1 = sil_1 \times e_1$ $sip_2 = sil_2 \times e_1$ sip₂: (0.0227)8.4727 $-0.4164)_{\alpha}$ The second lowest strain planes based on e2 can be similarly derived: $sip_3 = sil_3 \times e_2$ sip3: (-2.1084 5.6087 $1.5698)_{\alpha}$ sip4: (-2.0960 -5.582 $-1.5885)_{\alpha}$ $sip_4 = sil_4 \times e_2$

Step 2: Determine the crystal planes with minimum strain and minimum atomic movement

Now we need to go beyond PTMC by considering the atomic movement in the phase transition. The possible sip_i only takes into account the lattice strain between two connecting phases but the atomic match at the interface cannot be quantitatively measured. For diffusionless Martensitic phase transition, it is important that the atoms at the phase junction are closely matched and thus the atomic displacement needs to be as small as possible from one phase to another.

Based on the atom correspondence from the pathway obtained from SSW, we can search for the crystal plane with minimum strain and minimum atomic movement.

- a. The minimum strain condition is first utilized to screen the possible crystal Miller planes by minimizing the dihedral angle between the crystal plane ((hkl) with integer number) and the *sip_i*.
- b. The atomic movement can be calculated by summing the displacement of each atom from initial to the final phase while projecting out those due to rigid-body rotation.

The atomic movement is composed of two types of movement, parallel to the crystal plane (hkl) and perpendicular to the plane, d^{\perp} . For Martensitic phase transition, the phase transition is achieved often via slipping or twinning and thus the atomic movement needs to be dominated by those parallel to the habit plane.

In **P-II** of α - ω phase transition, if limiting the search within low index planes (**hkl**) with the absolute value of h, k, l being 0 or 1. Two solutions corresponding to *sip_i*, i=1, 2 are yielded:

SOLUTION 1: $(001)_{\alpha}$ plane, which is 9.08 degrees (**angle**) off *sip*₁. The atomic movement is 1.80 Å parallel to the plane and 2.80 Å perpendicular to the plane (**d**^{\perp}).

SOLUTION 2: $(010)_{\alpha}$ plane, which is 7.48 degrees off *sip*₂. The atomic movement is 2.94 Å parallel to the plane and 1.36 Å perpendicular to the plane.

The **SOLUTION 2**, $(010)_{\alpha}$, has the smallest \mathbf{d}^{\perp} (1.36 Å). By switching to the notation in conventional Bravais lattice, $(010)_{\alpha}$ is $(\mathbf{1\overline{100}})_{\alpha}$

The solutions for the second lowest strain planes are as follows:

SOLUTION 3: $(\bar{1}11)_{\alpha}$ plane, which is 24.84 degrees off *sip*₃. The atomic movement is 2.66 Å parallel to the plane and 2.04 Å perpendicular to the plane.

SOLUTION 4: $(111)_{\alpha}$ plane, which is 24.56 degrees off *sip₄*. The atomic movement is 2.66 Å parallel to the plane and 2.04 Å perpendicular to the plane.

We note that $(\overline{1}11)_{\alpha}$ and $(111)_{\alpha}$ are the same plane for α phase in the lattice of P-II. By switching to the notation in conventional Bravais lattice, $(111)_{\alpha}$ is $(1\overline{1}01)_{\alpha}$

Step 3: Identify the atomic habit plane (interface)

Finally, we utilize the determined possible atomic habit planes to establish the interface between two phases (see Figure S4). An atomic habit plane needs to exhibit a coherent interface between two phases, i.e. with the lowest interfacial energy.

For **P-II** in α - ω phase transition, we have two likely interfaces as suggested from Step 2: $(10\overline{1}0)_{\alpha}$ // $(1\overline{1}00)_{\omega}$ and $(1\overline{1}01)_{\alpha}$ // $(01\overline{1}1)_{\omega}$. $(10\overline{1}0)_{\alpha}$ // $(10\overline{1}0)_{\omega}$ has both minimum strain and minimum d[⊥]. By manually joining the two surfaces of the two phase together, we found that $(10\overline{1}0)_{\alpha}$ // $(1\overline{1}00)_{\omega}$ pair can form a coherent interface between the two phases. The DFT optimized interface is shown in the Figure S5 (d) with a low interfacial energy, 4 meV/Å². We therefore conclude that $(10\overline{1}0)_{\alpha}$ // $(1\overline{1}00)_{\omega}$ is the atomic habit plane and the OR can be written as $(10\overline{1}0)_{\alpha}$ // $(1\overline{1}00)_{\omega}$; $[0001]_{\alpha}$ // $[11\overline{2}0]_{\omega}$, which is equivalent to UZ Variant-II OR in literature.

Using the same approach, the OR and atomic planes (HP) for **P-I** could also be established. The e, I and *sil* and *sip* as defined in **Part 4** are listed in Table SIII below. Unlike that in **P-II**, we found that *sip*₁ and *sip*₂ have minimum strain but with large d^{\perp} , but *sip*₃ and *sip*₄ has a larger strain but with small d^{\perp} . In particular, *sip*₄ has a diminished d^{\perp} . By constructing these interfaces involving *sip*₄ and *sip*₂ in the superlattice, namely, $(11\overline{2}2)_{\alpha}//(1\overline{1}00)_{\omega}$ and $(\overline{1}2\overline{1}1)_{\alpha}//(1\overline{1}00)_{\omega}$, we found that $(11\overline{2}2)_{\alpha}//(1\overline{1}00)_{\omega}$ from *sip*₄ can achieve a stable

interface, while the $(\overline{1}2\overline{1}1)_{\alpha}/((\overline{1}00)_{\omega})$ from sip_2 is not stable, the optimization of which leads to pure phase. The structure of these interfaces are shown in Figure S5. The atomic habit plane is therefore determined as $(11\overline{2}2)_{\alpha}/((1\overline{1}00)_{\omega})$ with OR as $(11\overline{2}2)_{\alpha}/((1\overline{1}00)_{\omega})$; $[1\overline{1}00]_{\alpha}/[(11\overline{2}0]_{\omega})$, which is equivalent to UZ Variant-I OR in literature.

P-I		Note
e ₁	(0.4200 -0.3419 -0.8407)	
e ₂	(0.8878 0.3471 0.3024)	
e3	(0.1884 -0.8733 0.4492)	
I	0.80745	
I_2	0.97747	
I ₃	1.23083	
silı	(0.4371 -0.8414 -0.3178)	(on the plane defined by) $\mathbf{e}_1 \times \mathbf{e}_3$
sil ₂	(-0.183 -0.3365 0.9237)	$\mathbf{e}_1 \times \mathbf{e}_3$
sil ₃	(0.9036 0.0708 0.4226)	$\mathbf{e}_2 \times \mathbf{e}_3$
sil4	(-0.7912 -0.5917 -0.1546)	$\mathbf{e}_2 \times \mathbf{e}_3$
		*(hkl) angle d⊥
<i>sip</i> 1	(-0.8684 -1.6743 5.4062)	(001) 26.0° 2.3325
sip ₂	(-2.5451 5.3912 -1.6406)	$(1\overline{1}0)$ 28.73° 2.3230
sip3	(0.5117 4.4018 -4.4553)	$(0\overline{1}1)$ 5.22° 1.5259
sip4	(2.6790 -4.7318 4.6542)	(111) 19.91° 0.0059
Two likely interfaces	$(11\overline{2}2)_{\alpha}//(1\overline{1}00)_{\omega}; (sip_4)$	(a) and (b) in Figure S5
	$(\overline{1}2\overline{1}0)_{\alpha}//(1\overline{1}00)_{\omega}(sip_2)$	
Atomic HP	$(11\bar{2}2)_{\alpha}//(1\bar{1}00)_{\omega}$	
OR	$(11\bar{2}2)_{\alpha}//(1\bar{1}00)_{\omega}; [1\bar{1}00]_{\alpha}//[11\bar{2}0]_{\omega}$	

Table SIII. The OR and atomic habit planes (HP) for P-I (the structures are listed in Part 7). The e, I, *sil* and *sip* are as defined in Part 4.

*(hkl) is with respect to the lattice from the P-I pathway, not the conventional Bravais lattice.





Figure S5. Six possible α - ω heterophase junctions (HJ) created from P-I (a-c) and P-II (d-f). (a) $(11\overline{2}2)_{\alpha}/((1\overline{1}00)_{\omega})$ (the most stable interface of P-I, HJ-I, also see Figure 2c; (b) $(\overline{1}2\overline{1}1)_{\alpha}/((1\overline{1}00)_{\omega})$; (c) $(0001)_{\alpha}/((01\overline{1}1)_{\omega})$ (interface suggested from the first condition of Tao-1 OR); (d) $(10\overline{1}0)_{\alpha}/((1\overline{1}00)_{\omega})$ (the most stable HJ of P-II, HJ-II, also see Figure 2c; (e) $(1\overline{1}01)_{\alpha}/((01\overline{1}1)_{\omega})$ (f) $(0001)_{\alpha}/((11\overline{2}0)_{\omega})$ (interface suggested from the first condition of Silcock OR, HJ-III in Figure 2c) at hydrostatic pressure of 3 GPa. From our DFT calculations using the superlattice approach, the interface (a), (d-f) can be optimized as stable interfaces with mixed phases, and the other interfaces are not stable, falling back to pure phases after optimization. The calculated interfacial energy is 20 meV/Å² for the HJ-II in (a), 4 meV/Å² for the HJ-II in (d), 33 meV/Å² for the interface in (e) and 8 meV/Å² for the HJ-III in (f). The interfacial atoms are yellow colored.

The interfacial energy γ_{int} is calculated using Eq. S4.

 $\gamma_{\text{int}} = [E(\text{biphase}) - \Sigma_i n_i E_i(\text{pure phase})] / 2A$

(S4)

where E(biphase) is the total energy of the biphase crystal (superlattice), E_i (pure phase) is the energy of pure phase, n_i is number of Zr of the different phase components in the biphase and A is the surface area of the interface. Obviously, the lower γ_{int} is, the more stable the interface will be. In this work, all the interfaces in superlattice contain the same number of atoms in α and in ω phase (half-half composition).

In Table SIV, we listed the calculated elastic constants of pure α , ω phases, and the heterophase junctions, HJ-I and HJ-II in superlattice (Figure 2c). In general, our DFT results agree with the experimental values and the previous calculations at zero pressure for pure phases. The B/G ratio is related to the brittleness (ductility) of material. A large B/G value indicates a high ductility, while a low value reflects the brittleness. It is seen from Table SIV that the HJ-I from P-I (OR-I, Figure 2c and Figure S5-a) has a larger B/G value than pure α and ω phase, while HJ-II from P-II (OR-II, Figure 2c and Figure S5-d) has a smaller B/G value than pure phases. It shows that HJ-II from P-II would be more brittle than pure zirconium.

		В	G	B/G
	This work (3GPa)	102.6	38.2	2.69
Pure a	This work (0GPa)	97.4	34.1	2.85
	Expt.	97.6^{36} 94^{37} 95.3^{38}	36.138	
	Other works (0GPa)	93.4 ³⁹ 97.1 ⁴⁰ 99.8 ⁴¹ 97.5 ⁴²		
	This work (3GPa)	104.0	50.5	2.06
Pure ω	This work (0GPa)	97.6	45.3	2.15
	Expt	90.0 ³⁷ 109.0 ³⁷ 104.0 ⁴³	45.1 ⁴³	
	Other works (0 GPa)	101.1 ³⁹		
HJ-I	This work (3GPa)	96.6	28.8	3.35
(Fig. 2)				
HJ-II	This work (3GPa)	108.0	53.4	2.02
(Fig. 2)				

Table SIV: Bulk modulus (B), shear modulus (G) and B/G ratio for pure α , ω phase and the mixed phase junctions of zirconium at 3 GPa.

References

- 1 M. P. Usikov and V. A. Zilbershtein, Phys. Stat. Sol. (a), 1973, 19, 53-58.
- 2 A. Rabinkin, M. Talianker and O.Botstein, Acta Metall, 1980, 29, 691-698.
- 3 A. R. Kutsar, I. V. Lyasotski, A. M. Podurets and A. F. Sanches-bolinches, *High Pressure Res*, 1990, 4, 475-477.
- 4 S. G. Song and G. T. Gray, *Philos. Mag. A*, 1995, 71, 275-290.
- 5 G. Jyoti, K. D. Joshi, S. C. Gupta and S. K. Sikka, Philos. Mag. Lett, 1997, 75, 291-300.
- 6 D. R. Trinkle, R. G. Hennig, S. G. Srinivasan, D. M. Hatch, M. D. Jones, H. T. Stokes, R. C. Albers and J. W. Wilkins, *Phys. Rev. Lett*, 2003, **91**, 025701-025704.
- 7 E. Cerreta, G. T. Gray, R. S. Hixson, P. A. Rigg and D. W. Brown, Acta Mater, 2005, 53, 1751-1758.
- 8 G. Jyoti, R. Tewari, K. D. Joshi, D. Srivastava, G. K. Dey, S. C. Gupta, S. K. Sikka and S. Banerjee, *Defect Diffus. Forum*, 2008, 279, 133-138.
- 9 H. R. Wenk, P. Kaercher, W. Kanitpanyacharoen, E. Zepeda-Alarcon and Y. Wang, *Phys. Rev. Lett*, 2013, 111, 195701-195705.
- 10 H. Zong, T. Lookman, X. Ding, S.-N. Luo and J. Sun, Acta Mater, 2014, 65, 10-18.
- 11 H. Zong, T. Lookman, X. Ding, C. Nisoli, D. Brown, S. R. Niezgoda and S. Jun, Acta Mater, 2014, 77,

191-199.

- 12 C. Shang and Z. P. Liu, J. Chem. Theory Comput, 2013, 9, 1838-1845.
- 13 X. J. Zhang, C. Shang and Z. P. Liu, J. Chem. Theory Comput, 2013, 9, 3252-3260.
- 14 C. Shang, X. J. Zhang and Z. P. Liu, Phys. Chem. Chem. Phys., 2014, 16, 17845-17856.
- 15 X.-J. Zhang, C. Shang and Z.-P. Liu, J. Chem. Theory Comput, 2013, 9, 5745-5753.
- 16 C. Shang and Z. P. Liu, J. Chem. Theory Comput., 2012, 8, 2215-2222.
- 17 C. Shang and Z.-P. Liu, J. Chem. Theory Comput., 2010, 6, 1136-1144.
- 18 G. Kresse and J. Furthmüller, *Phys. Rev. B*, 1996, **54**, 11169-11186.
- 19 G. Kresse and J. Furthmüller, Comput. Mater. Sci, 1996, 6, 15-50.
- 20 P. E. Blöchl, Phys. Rev. B, 1994, 50, 17953-17979.
- 21 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett*, 1998, 80, 891.
- 22 G. Kresse, J. FurthmüLler and J. Hafner, *Europhys.Lett*, 1995, **32**, 729-734.
- 23 W. Frank, C. Elsässer and M. Fähnle, *Phys Rev Lett*, 1995, 74, 1791-1794.
- 24 A. Togo, F. Oba and I. Tanaka, *Phys. Rev. B*, 2008, 78, 134106.
- 25 Y. Le Page and P. Saxe, *Physical Review B*, 2002, 65.
- 26 N. W. Ashcroft and N. D. Mermin, *Philadelphia: Saunders College*, 1976.
- 27 Z. Sun, S. Li, R. Ahuja and J. M. Schneider, Solid State Communications, 2004, 129, 589-592.
- 28 E.Schreiber, O.L.Anderson and N.Soga, New York: Mcgraw-Hill, 1973.
- 29 J. S. Bowles and J. K. Mackenzie, Acta Metall, 1954, 2, 129-137.
- 30 J. K. Mackenzie and J. S. Bowles, Acta Metall, 1954, 2, 138-147.
- 31 G. K. Bansal and A. H. Heuer, Acta Metall, 1974, 22, 409-417.
- 32 M.S.Wechsler and T.A.Lieberman, Trans.Am.Inst.Min.Engrs, 1953, 197, 1503-1515.
- 33 C. M. Wayman, New York: Macmillan Co., 1964, 76-80.
- 34 C. M. Wayman, J. Less-Common Metals, 1972, 28, 97-105.
- 35 X. L. Xiao, C. P. Luo and J. W. liu, Sci. China, Ser. E, 2002, 45, 58-64.
- 36 B. Olinger and J. C. Jamieson, *High Temp.High Pressures*, 1973, 5, 123-131.
- Y. Zhao, J. Zhang, C. Pantea, J. Qian, L. L. Daemen, P. A. Rigg, R. S. Hixson, G. T. Gray, Y. Yang, L. Wang,
 Y. Wang and T. Uchida, *Phys. Rev. B*, 2005, **71**, 184119-184124.
- 38 E. S. Fisher, J Appl Phys, 1970, 41, 2991.
- 39 Y. J. Hao, L. Zhang, X. R. Chen, Y. H. Li and H. L. He, J. Phys. : Condens. Matter, 2008, 20, 235230.
- 40 D. J. OH and R. A. Johnson, J.Nucl.mater, 1989, 169, 5-8.
- 41 F. Willaime and C. Massobrio, *Phys Rev B*, 1991, **43**, 11653-11665.
- 42 F. Cleri and V. Rosato, *Phys Rev B*, 1993, **48**, 22-33.
- 43 W. Liu, B. Li, L. Wang, J. Zhang and Y. Zhao, *Phys Rev B*, 2007, 76, 144107-144110.

Part 6 The Cartesian atomic coordinates for P-I, P-II, P(HJ-I) and P(HJ-II)

P-I			
α-phase	a=6.0497	b=5.5458 c=5.5456	α=120° β=90° γ=117°
	Х	Y	Z
	2.104591	-0.47915	1.909945
	0.421708	1.771182	3.438113
	4.28239	1.68907	1.146356
	1.257478	2.206195	0.381911
	3.446659	1.253685	4.202805

	5.129516	-0.9962	2.674263
TS1	a=5.913 b=5.7275	c=5.727 α =124° β =90	° γ=116°
	Х	Υ	Z
	2.319818	-0.73684	1.612058
	0.665882	1.855359	3.286472
	4.150509	1.736862	1.350145
	1.216924	1.950416	0.345753
	3.360321	0.752764	4.186863
	5.252898	-0.95056	2.615626
ω-phase	a=5.901 b=5.898	c=5.898 α =130° β =85°	γ=116°
	Х	Y	Z
	2.398665	-0.8832	1.444625
	1.102164	1.764549	2.888627
	4.052608	1.76527	1.444602
	1.102689	1.765681	-0.00052
	3.224138	0.440576	4.334394
	5.348572	-0.88361	2.889734
P-II			
α-phase	a=5.131 b=8.489	c=3.202 α =101° β =90	ο° γ=90°
	Х	Y	Z
	8.119898	-0.40799	4.546797
	0.436148	9.892251	4.882902
	8.137671	11.72593	0.35479
	8.135627	13.53628	5.594255
	0.44223	13.53678	0.692574
	0.438615	15.34737	5.93141
TS2	a=5.052 b=8.514	$c=3.167$ $\alpha=95^{\circ}$ $\beta=90^{\circ}$	γ=90 °
	Х	Y	Ζ
	2.938924	0.539731	1.488119
	0.413742	2.143765	1.714288
	2.938901	3.511379	0.128684
	2.938907	6.116012	2.002049
	0.41379	5.084719	1.198786
	0.413914	16.20388	3.073626
ω-phase	a=5.007 b=8.669	$c = 3.120 \alpha = 90^{\circ} \beta = 90^{\circ}$	ο γ=90°
	Х	Y	Z
	7.927614	0.723208	4.679804
	0.417259	10.83581	4.681728
	7.92759	12.2811	1.92E-05
	7.927611	15.17029	4.680914
	0.417247	13.72662	1.55897
	0.417267	16.61582	6.240539
P(HJ-I)	a= 16.475 b= 6.033	$c=5.531$ $\alpha=90.7^{\circ}$ $\beta=90$).2° γ=83.8°

Х	Y	Z
0.596206	5.440224	5.10589
0.271105	2.508434	0.447855
7.234932	3.474308	3.21249
6.923107	0.477126	2.340986
5.649523	1.442836	5.105378
5.981729	4.508243	0.447226
4.707818	5.472753	3.213205
4.397375	2.475438	2.34047
2.777741	0.441366	5.977867
3.143753	3.509414	-0.42453
1.869878	4.475319	2.339891
1.524264	1.475502	3.212639
8.833636	5.440224	5.10589
8.508577	2.508434	0.447855
15.47236	3.474309	3.21249
15.16053	0.477126	2.340987
13.88695	1.442837	5.105378
14.21916	4.508243	0.447225
12.94525	5.472753	3.213205
12.6348	2.475438	2.34047
11.03636	0.509444	0.447026
11.35999	3.441336	5.106309
10.10731	4.475319	2.339891
9.761693	1.475502	3.212639
a= 17.286	b= 6.142 c= 5.106 α = 90.1°	$3=90.0^{\circ} \gamma=90.9^{\circ}$
Х	Y	Ζ
-0.07069	5.195743	4.972417
-0.02198	2.130447	0.157564
7.102177	3.689735	2.69801
7.148772	0.619862	2.432735
5.729693	1.980345	4.973431
5.685505	5.055846	0.156849
4.25797	5.2352	2.701828
4.304609	2.16464	2.428161
2.876578	0.517628	5.133497
2.832826	3.593359	-0.0033
1.358208	5.016387	2.427177
1.404722	1.94618	2.702846
8.593499	5.640945	4.885926
8.642254	2.57586	0.243893
15.85037	3.492133	2.698005
15.89735	0.422249	2.4325
14.35018	1.527956	4.88755

 α -phase

ts1

	14.30588	4.603547	0.242974
	12.88758	5.643269	2.815392
	12.93516	2.573375	2.314638
	11.52034	0.516325	0.253651
	11.4724	3.58175	4.87678
	10.02003	4.615441	2.315279
	10.06575	1.544787	2.814879
HJ-I (int1)	a= 17.412 b= 6.	165 c= 5.052 α = 90.0°	$\beta = 90.0^{\circ} \gamma = 91.9^{\circ}$
	Х	Y	Ζ
	-0.16706	5.148065	4.979498
	-0.06644	2.067648	0.093026
	7.082114	3.731736	2.634716
	7.182697	0.651459	2.438065
	5.743924	2.06438	4.980431
	5.643333	5.144336	0.091983
	4.185471	5.199405	2.604972
	4.286242	2.118273	2.467232
	2.890443	0.525514	5.037214
	2.789523	3.60581	0.034915
	1.292942	5.093111	2.466788
	1.393613	2.01239	2.605652
	8.556604	5.663427	4.85557
	8.657447	2.582894	0.217529
	15.91154	3.480148	2.635339
	16.01257	0.399502	2.437487
	14.42754	1.537247	4.855817
	14.32709	4.618039	0.217018
	12.87962	5.669091	2.764449
	12.9804	2.588475	2.308339
	11.59264	0.516747	0.232458
	11.49199	3.597296	4.840311
	10.01588	4.631645	2.309625
	10.11642	1.551017	2.763364
s2	a= 17.400 b= 6.	171 c= 5.046 α = 90.0°	$\beta = 90.0^{\circ} \gamma = 91.8^{\circ}$
	Х	Y	Ζ
	-0.15543	5.163301	4.98104
	-0.06104	2.079392	0.085442
	7.10411	3.70264	2.618011
	7.19844	0.618721	2.448648
	5.740683	2.05392	4.98425
	5.646086	5.137847	0.082212
	4.195485	5.18983	2.592925
	4.290062	2.105893	2.473472
	2 889992	0.52507	5.028168

 2.795279		3.60911	12		0.038113	
1.30209		5.11215	53		2.47122	
1.396579		2.02816	52		2.595215	
8.55678		5.57677	77		4.837229	
8.651476		2.49285	58		0.229743	
15.88992		3.51300)4		2.622489	
15.98474		0.42905	52		2.444093	
14.41095		1.59989	98		4.834134	
14.31659		4.68401	15		0.232526	
12.88602		5.62899	95		2.771539	
12.98042		2.54503	39		2.294927	
11.57544		0.52283	31		0.210403	
11.48094		3.60673	33		4.855955	
10.01523		4.71804	42		2.297718	
10.10937		1.63406	57		2.768957	
a= 17.455	b= 6.223	c= 4.992	α= 90.0°	β= 90.0°	γ=90.2°	
Х		Y			Ζ	
17.40834		5.23160)6		4.954732	
17.41846		2.12000	01		0.05731	
7.26359		3.65284	18		2.499564	
7.273555		0.54127	76		2.513082	
5.811574		2.09388	38		0.004317	
5.801621		5.20540)3		0.016236	
4.356819		5.20329	97		2.512798	
4.366812		2.09179	98		2.499802	
2.915242		0.52664	42		0.004289	
2.905277		3.63816	51		0.016154	
1.470849		5.17060)9		2.470509	
1.480875		2.05908	39		2.541748	
8.68752		5.2224	9		4.972199	
8.697542		2.11077	74		0.040369	
16.09543		3.59191	18		2.589427	
16.10549		0.48042	25		2.42247	
14.47016		1.45137	76		4.824495	
14.46011		4.56280)6		0.187544	
13.15713		5.82324	47		2.684365	
13.16706		2.7116	7		2.327697	
11.54021		0.56869	98		0.093417	
11.53014		3.68028	33		4.918644	
10.20815		5.15828	37		2.463813	
10.21811		2.04679	94		2.54851	
a= 17.413	b= 6.216	c= 5.007	α= 90.0°	β= 90.0°	γ=90.6°	
Х		Y			Ζ	
17.39039		5.24519	96		4.969817	

int2

17.40889 2.134749 0.065631 7.247983 3.667958 2.506872 7.272801 0.558782 2.527348 5.80782 2.095989 0.000927 5.778146 5.20529 0.026081 4.336782 5.215351 2.528387 4.359329 2.105794 2.50336 2.997682 0.534716 0.002618 2.802558 3.643168 0.02774 1.44066 5.171654 2.478552 1.462213 2.06244 2.55659 8.676365 5.249728 4.981347 8.697751 2.14066 0.02552 1.60401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06037 5.658415 2.726913 13.0637 5.658415 2.726913 13.06037 5.658415 2.72691 13.06037 5.658415 2.72691				
0247983 3.667958 2.506872 7.272801 0.558782 2.527348 5.800782 2.095989 0.000927 5.778146 5.20529 0.020681 4.336782 5.215351 2.528387 4.339329 2.105794 2.50336 2.917682 0.534716 0.002618 2.892658 3.643168 0.023774 1.44066 5.171654 2.478552 1.6602785 0.487171 2.438967 1.440063 5.5249738 4.812158 1.440063 1.661456 4.812158 1.462213 2.06244 2.55723 1.600785 0.487171 2.438967 1.442023 1.661456 4.812158 1.449033 1.661456 4.812158 1.449033 5.658415 2.769131 3.06037 5.658415 2.70813 1.56443 3.721316 4942311 0.14288 5.27718 2.56722 1.572437 2.090662 0.010467		17.40889	2.134749	0.065631
0.558782 2.527348 5.800782 2.095989 0.000927 5.778146 5.20529 0.026081 4.3359329 2.105794 2.523337 4.359329 2.105794 2.50336 2.917682 0.534716 0.002618 2.892658 3.643168 0.023774 1.440261 2.05244 2.55659 8.676365 5.249738 4.981147 8.697751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06371 5.658415 2.726913 13.06373 5.658415 2.726913 13.08343 2.548262 2.308874 11.57624 0.612507 0.09309 11.57643 5.183737 2.46004 10.16407 2.075118 2.56772 2.42096 5.022379 5.242496 5.02379		7.247983	3.667958	2.506872
 5.800782 2.095989 0.000927 5.778146 5.20529 0.026081 4.336782 5.215351 2.528336 2.917682 0.534716 0.002618 2.892658 3.643168 0.023774 1.44066 5.171654 2.478552 1.462213 2.06244 2.55659 8.676365 5.249738 4.981347 8.697751 2.14066 0.023521 1.60401 3.596987 2.597801 1.60455 4.812158 1.449023 1.661456 4.812158 1.449023 1.661456 4.812158 1.447348 4.771319 0.223521 1.306037 5.658415 2.726913 1.306343 2.548262 2.308874 1.57624 0.612507 0.99309 11.55443 3.721316 4.940231 10.14288 5.183737 2.468044 10.16407 2.507511 2.900° (F 90.0° 790.1° 790.1° 790.1° 790.1° 790.1° 790.1° 791.2 2.51674 3.67192 2.51674 3.67035 3.67035<!--</td--><td></td><td>7.272801</td><td>0.558782</td><td>2.527348</td>		7.272801	0.558782	2.527348
5.778146 5.20529 0.026081 4.336782 5.215351 2.528387 4.359329 2.105794 2.50336 2.917682 0.534716 0.002618 2.892658 3.643168 0.023774 1.44066 5.171654 2.478552 1.462213 2.06244 2.55639 8.676365 5.249738 4.981347 8.697751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06037 5.568415 2.726913 13.08343 2.548262 2.30874 11.55624 0.612507 0.099039 11.5543 3.721316 4.942311 10.14288 5.183737 2.468094 10.16407 2.075118 2.50772 2.917257 5.242496 5.022379 17.25679 2.104703 0.009786		5.800782	2.095989	0.000927
 4.336782 5.215351 2.528387 4.359329 2.105794 2.50336 2.917682 0.534716 0.0023774 1.44066 5.171654 2.478552 1.462213 2.06244 2.55659 8.676365 5.249738 4.981347 8.697751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.47348 4.7171319 0.22352 13.06037 5.658415 2.726913 13.08343 2.548262 2.308874 11.57624 0.612507 0.093039 11.55443 3.721316 4.942311 10.14288 5.183737 2.46804 10.16407 2.075118 2.56772 a=17.253 b=6.273 c=5.013 a=90.0° p=90.1° x x Y 2.56772 2.31674 3.67192 2.516743 7.193374 3.67192 2.516743 7.193374 3.67192 2.516743 7.193374 3.67192 2.516743 7.193374 3.67192 2.516743 2.480755 3.670058 0.009865 3.436705 2.516891 1.438631 5.237213 0.010466 3.237569 2.516827 3.670058 0.009885 3.670058 0.009885 3.670058 0.009885 3.670058 0.009885 3.670058 0.0		5.778146	5.20529	0.026081
 4.359329 2.105794 2.50336 2.917682 0.534716 0.002618 2.892658 3.643168 0.023774 1.44066 5.171654 2.455659 8.676365 5.249738 4.981347 8.697751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.4871711 2.438967 14.47023 1.661456 4.812158 1.447348 4.771319 0.22352 13.06037 5.658415 2.726913 13.06037 5.183737 2.468094 10.16407 2.075118 2.56772 2.104703 0.009786 7.193374 3.67192 2.516143 7.19321 5.237213 0.010467 5.749321 5.237213 0.0104664 2.51594 4.316769 5.242496 5.023379 1.43851 5.237569 2.516827 8.63053 2.104703 0.009855 1.43881 5.237569 2.516827 8.63053 2.104701 0.009875 1.54963 3.671019 2.516827 <l< td=""><td></td><td>4.336782</td><td>5.215351</td><td>2.528387</td></l<>		4.336782	5.215351	2.528387
2.917682 0.534716 0.002618 2.892658 3.643168 0.023774 1.44066 5.171654 2.478552 1.462213 2.06244 2.55659 8.676365 5.249738 4.981347 8.67751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06037 5.568415 2.726913 13.08343 2.548262 2.08974 11.57624 0.612507 0.093039 11.55443 3.721316 4.942311 10.14288 5.183737 2.468094 10.16407 2.075118 2.56772 x Y Z 7.1725679 2.104703 0.009786 7.19374 3.67192 2.516743 7.19661 0.534603 2.51618 5.72437 2.099662 0.010467 5.749321		4.359329	2.105794	2.50336
2.892658 3.643168 0.023774 1.44066 5.171654 2.478552 1.462213 2.06244 2.55659 8.676365 5.249738 4.981347 8.697751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.49023 1.661456 4.812158 14.49023 1.661456 4.812158 13.06037 5.658415 2.726913 13.08343 2.548262 2.308874 11.57624 0.612507 0.093039 11.55443 3.721316 4942311 10.14288 5.183737 2.468094 10.16407 2.075118 2.56772 2 17.25877 5.242496 5.022379 17.25877 5.242496 5.022379 17.25679 2.104703 0.009786 7.193374 3.67192 2.516743 7.19661 0.534603 2.51618 <th></th> <th>2.917682</th> <th>0.534716</th> <th>0.002618</th>		2.917682	0.534716	0.002618
 n.44066 5.171654 2.478552 1.462213 2.06244 2.55659 8.676365 5.249738 4.981347 8.697751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.4871711 2.438967 14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06037 5.658415 2.726913 13.08343 2.548262 2.308874 11.57624 0.612507 0.093039 11.55443 3.721316 4.942311 10.14288 5.183737 2.468094 10.16407 2.075118 2.66772 a = 17.253 b 6.273 c 5.013 a -90.0° p-90.0° p-01.° X Y Z 17.25877 5.242496 5.022379 17.25679 2.104703 0.009786 7.193374 3.67192 2.516743 2.104664 2.51594 4.319908 2.104664 2.51594 4.319908 2.104664 2.51594 4.319908 2.104664 2.51585 2.880755 0.534625 0.010463 2.87599 3.670058 0.009885 1.43863 2.104701 0.0097		2.892658	3.643168	0.023774
1.4622132.062442.556598.6763655.2497384.9813478.697512.140660.0525216.004013.5969872.59780116.027850.4871712.43896714.490231.6614564.81215814.473484.7713190.2235213.060375.6584152.72691313.083432.5482622.30887411.576240.6125070.09303911.554433.7213164.94231110.142885.1837372.46809410.164072.0751182.56772α = 17.253b = 6.273c = 5.013α = 17.253b = 6.273c = 5.013α = 17.25375.2424965.02237917.256775.2424965.02237917.256775.2421452.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104675.7493215.2372130.0104664.3197082.1019052.5168271.438315.2375692.5168278.6305333.6719192.5167428.6305333.6719192.5167428.6305333.6719192.5167428.6305333.6719192.5167428.6305333.6719192.5167428.6305333.6719192.5167428.6305333.6719192.516742<		1.44066	5.171654	2.478552
8.6763655.2497384.9813478.6977512.140660.0525216.004013.5969872.59780116.027850.4871712.43896714.490231.6614564.81215814.473484.7713190.2235213.060375.6584152.72691313.083432.5482622.30887411.576240.6125070.09303911.554433.7213164.94231110.142885.1837372.46809410.164072.0751182.56772a=17.253b=6.273c=5.013a=90.0°β=90.0°γ=90.1°xYZ17.258775.2424965.02237917.258792.1047030.0097867.1933743.671922.5167437.19610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104675.7493215.2372130.0104664.3167695.2421452.516891.4388315.2375692.516891.4388315.2375692.516891.4388315.2375692.5168278.6305532.1047010.00978515.819633.6710192.51674215.82870.5346042.51618115.82870.5346042.51618115.819633.6719192.51674215.82870.5346042.		1.462213	2.06244	2.55659
8.697751 2.14066 0.05252 16.00401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06037 5.658415 2.726913 13.08343 2.548262 2.308874 11.57624 0.612507 0.093039 11.55443 3.721316 4.942311 10.14288 5.183737 2.468094 10.16407 2.075118 2.56772 a=17.253 b=6.273 c=5013 a=90.0° p=90.1° X Y Z 7.17.25877 5.242496 5.022379 17.25679 2.104703 0.009786 7.193374 3.67192 2.516743 7.19661 0.534603 2.516118 5.752437 2.099662 0.010467 5.749321 5.237213 0.010466 4.316769 5.242145 2.515985 2.860755 0.534325 0.010466 2.515985 2.86353 2.516		8.676365	5.249738	4.981347
16.00401 3.596987 2.597801 16.02785 0.487171 2.438967 14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06037 5.658415 2.726913 13.08343 2.548262 2.308874 11.57624 0.612507 0.093039 11.55443 3.721316 4.942311 10.14288 5.183737 2.468094 10.16407 2.075118 2.56720 0.0-phase a=17.253 b=6.273 c=5013 α=90.0° β=90.0° X Y Z 7 7 2.468094 10.16407 2.075118 2.56775 1 X Y Z 7 7.125679 2.104703 0.009786 7.193374 3.67192 2.516743 7.19661 0.534603 2.51618 5.752437 2.099662 0.010466 4.316769 5.242145 2.515985 2.880755 0.534325 <td< td=""><td></td><td>8.697751</td><td>2.14066</td><td>0.05252</td></td<>		8.697751	2.14066	0.05252
16.027850.4871712.43896714.490231.6614564.81215814.473484.7713190.2235213.060375.6584152.72691313.083432.5482622.30887411.576240.6125070.09303911.554433.7213164.94231110.142885.1837372.46809410.164072.0751182.56772∞-phasea=17.253b=6.273c= 5.013a=90.0°β=90.0°XYZ17.258775.2424965.02237917.256792.1047030.0097867.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759553.6700580.0098851.4388315.2375692.516821.436932.1019052.516821.436932.1019052.516821.436932.1019052.516821.5819633.6719192.51674215.819633.6719192.51674215.822870.5346042.51611814.35542.1018925.023062		16.00401	3.596987	2.597801
14.49023 1.661456 4.812158 14.47348 4.771319 0.22352 13.06037 5.658415 2.726913 13.08343 2.548262 2.308874 11.57624 0.612507 0.093039 11.55443 3.721316 4.942311 10.14288 5.183737 2.468094 10.16407 2.075118 2.56772 0.99hase a=17.253 b=6.273 c=5.013 a=90.0° γ=90.1° X Y Z 7 7 7 17.25877 5.242496 5.022379 7 17.25877 5.242496 5.022379 17.25679 2.104703 0.009786 7.196374 3.67192 2.516743 7.196374 5.237213 0.0104667 5.752437 2.099662 0.010467 5.759321 5.237213 0.0104663 2.880755 0.534325 0.010463 2.880755 0.534325 0.010463 2.863531 5.242496 <td< td=""><td></td><td>16.02785</td><td>0.487171</td><td>2.438967</td></td<>		16.02785	0.487171	2.438967
14.473484.7713190.2235213.060375.6584152.72691313.083432.5482622.30887411.576240.6125070.09303911.554433.7213164.94231110.142885.1837372.46809410.164072.0751182.56772∞-phasea=17.253b=6.273c=5.013a=90.0°β=90.0°XYZ17.256792.1047030.0097867.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.875953.6700580.0098851.4388315.2375692.5168278.6305532.1047010.0097861.438643.6719192.5167421.5.82870.5346042.5168278.6305532.1047010.0097851.5.81633.6719192.5167421.5.82870.5346042.51611814.385642.1018925.023062		14.49023	1.661456	4.812158
13.060375.6584152.72691313.083432.5482622.30887411.576240.6125070.09303911.554433.7213164.94231110.142885.1837372.46809410.164072.0751182.56772∞-phasea=17.253b=6.273c=5.013a=90.0°β=90.0°XYZ17.258775.2424965.02237917.256792.1047030.0097867.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.875953.6700580.0098851.4388315.2375692.5168278.6305532.1019052.5168278.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.5151814.385642.1018925.023062		14.47348	4.771319	0.22352
13.083432.5482622.30887411.576240.6125070.09303911.554433.7213164.94231110.142885.1837372.46809410.164072.0751182.56772a=17.253b=6.273c=5.013α=90.0°βa=17.253b=6.273c=5.013α=90.0°xYZ17.258775.2424965.02237917.256792.1047030.0097867.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515982.8807550.5343250.0104032.8807550.5343250.0104032.8807553.6700580.0098851.4388315.2375692.5168978.6325315.2424965.02237915.819633.6719192.51674215.819633.6719192.51674215.82870.5346042.51611815.819633.6719192.51674215.82870.5346042.51611814.35542.1018925.022379		13.06037	5.658415	2.726913
$ \begin{array}{c c c c c c c c c } & 0.612507 & 0.093039 \\ 11.55443 & 3.721316 & 4.942311 \\ 10.14288 & 5.183737 & 2.468094 \\ 10.16407 & 2.075118 & 2.56772 \\ a=17.253 & b=6.273 & c=5.013 & a=90.0^{\circ} & \beta=90.0^{\circ} & \gamma=90.1^{\circ} \\ \hline X & Y & Z \\ 17.25877 & 5.242496 & 5.022379 \\ 17.25679 & 2.104703 & 0.009786 \\ 7.193374 & 3.67192 & 2.516743 \\ 7.19661 & 0.534603 & 2.516118 \\ 5.752437 & 2.099662 & 0.010467 \\ 5.749321 & 5.237213 & 0.010466 \\ 4.316769 & 5.242145 & 2.51594 \\ 4.319908 & 2.104664 & 2.515985 \\ 2.880755 & 0.534325 & 0.010403 \\ 2.875995 & 3.670058 & 0.009885 \\ 1.438831 & 5.237569 & 2.51689 \\ 1.43693 & 2.101905 & 2.51689 \\ 1.43693 & 2.101905 & 2.51689 \\ 1.43693 & 2.101905 & 2.51689 \\ 1.43693 & 2.101905 & 2.51689 \\ 1.43693 & 2.101905 & 2.51689 \\ 1.43693 & 2.101905 & 2.51689 \\ 1.43693 & 2.101905 & 2.51689 \\ 1.438831 & 5.237569 & 2.51689 \\ 1.438831 & 5.237214 & 0.010465 \\ 1.438564 & 2.101892 & 5.023062 \\ 1.437557 & 5.237214 & 0.010465 \\ 1.438564 & 2.0101892 & 5.023062 \\ 1.437557 & 5.237214 & 0.010465 \\ 1.438564 & 2.0101892 & 5.023062 \\ 1.43757 & 5.237214 & 0.010465 \\ 1.438564 & 2.0101892 & 5.023624 \\ 1.438564 & 2.018892 & 5.023062 \\ 1.438564 & 5$		13.08343	2.548262	2.308874
11.554433.7213164.94231110.142885.1837372.46809410.164072.0751182.56772a=17.253b=6.273c=5.013a=90.0°XYZ17.258775.2424965.02237917.256792.1047030.0097867.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.875953.6700580.0098851.4388315.2375692.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51511814.385642.1018925.02306214.375575.2372140.010465		11.57624	0.612507	0.093039
00 -phase 10.14288 5.183737 2.468094 00 -phase $a = 17.253$ $b = 6.273$ $c = 5.013$ $a = 90.0^{\circ}$ $\beta = 90.0^{\circ}$ $\gamma = 90.1^{\circ}$ X Y Z 17.25877 5.242496 5.022379 17.25679 2.104703 0.009786 7.193374 3.67192 2.516743 7.19661 0.534603 2.516118 5.752437 2.099662 0.010467 5.749321 5.237213 0.0104664 4.316769 5.242145 2.51594 4.319908 2.104664 2.515985 2.880755 0.534325 0.010403 2.87595 3.670058 0.009885 1.438831 5.237569 2.516827 8.632531 5.242496 5.022379 8.630553 2.104701 0.009785 15.81963 3.671919 2.516742 15.82287 0.534604 2.516118 14.33564 2.101892 5.023062 14.37557 5.237214 0.010465		11.55443	3.721316	4.942311
		10.14288	5.183737	2.468094
∞ -phase $a = 17.253$ $b = 6.273$ $c = 5.013$ $a = 90.0^{\circ}$ $\beta = 90.0^{\circ}$ $\gamma = 90.1^{\circ}$ X Y Z 17.25877 5.242496 5.022379 17.25679 2.104703 0.009786 7.193374 3.67192 2.516743 7.19661 0.534603 2.516118 5.752437 2.099662 0.010467 5.749321 5.237213 0.010466 4.316769 5.242145 2.51594 4.319908 2.104664 2.515985 2.880755 0.534325 0.010403 2.875995 3.670058 0.009885 1.438831 5.237569 2.516897 1.443693 2.101905 2.516827 8.630553 2.104701 0.009785 15.81963 3.671919 2.516742 15.82287 0.534604 2.516118 14.38564 2.101892 5.023062 14.37557 5.237214 0.010465		10.16407	2.075118	2.56772
XYZ17.258775.2424965.02237917.256792.1047030.0097867.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.319082.1046642.5159852.8807550.5343250.0104032.8759553.6700580.0098851.4388315.2375692.5168971.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465	ω-phase	a=17.253 b=	6.273 c= 5.013 α = 90.0° β =	$=90.0^{\circ} \gamma = 90.1^{\circ}$
17.258775.2424965.02237917.256792.1047030.0097867.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759953.6700580.0098851.438315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		Х	Y	Ζ
17.256792.1047030.0097867.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759553.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		17.25877	5.242496	5.022379
7.1933743.671922.5167437.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759953.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		17.25679	2.104703	0.009786
7.196610.5346032.5161185.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759953.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		7.193374	3.67192	2.516743
5.7524372.0996620.0104675.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759953.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		7.19661	0.534603	2.516118
5.7493215.2372130.0104664.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759953.6700580.0098851.4388315.2375692.516891.436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		5.752437	2.099662	0.010467
4.3167695.2421452.515944.3199082.1046642.5159852.8807550.5343250.0104032.8759953.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		5.749321	5.237213	0.010466
4.3199082.1046642.5159852.8807550.5343250.0104032.8759953.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		4.316769	5.242145	2.51594
2.8807550.5343250.0104032.8759953.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		4.319908	2.104664	2.515985
2.8759953.6700580.0098851.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		2.880755	0.534325	0.010403
1.4388315.2375692.516891.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		2.875995	3.670058	0.009885
1.4436932.1019052.5168278.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		1.438831	5.237569	2.51689
8.6325315.2424965.0223798.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		1.443693	2.101905	2.516827
8.6305532.1047010.00978515.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		8.632531	5.242496	5.022379
15.819633.6719192.51674215.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		8.630553	2.104701	0.009785
15.822870.5346042.51611814.385642.1018925.02306214.375575.2372140.010465		15.81963	3.671919	2.516742
14.385642.1018925.02306214.375575.2372140.010465		15.82287	0.534604	2.516118
14.37557 5.237214 0.010465		14.38564	2.101892	5.023062
		14.37557	5.237214	0.010465
12 94302 5 242145 2 51594		12 0 12 02	5 242145	2 51504

	12.94616	2.104664			2.515985
	11.50701	0.534326			0.010404
	11.50921		3.6722	.85	5.022479
	10.06509		5.23757		2.516889
	10.06995		2.1019	04	2.516828
P(HJ-II)					
α-phase	a= 3.204	b= 5.137	c= 16.930	α= 90.0°	β= 100.8° γ=90.0°
-	Х		Y		Z
	0.004734		3.8525	91	0.92439
	1.60234		1.2842	22	1.847286
	0.004613		1.284221		4.619027
	1.611169		3.8525	89	3.695501
	0.013585		3.852589		6.467223
	1.611165		1.28422		7.390458
	-1.58364		3.852588		9.238135
	0.013948		1.284218		10.16191
	-1.5837		1.284219 3.852588 3.852587 1.284218		12.93352
	0.022808				12.01026
	-1.57483				14.78185
	0.022666				15.70509
ts4	a= 3.160	b= 5.105	c=17.385	α=90.0°	β = 103.4° γ =90.0°
	Х		Y		Z
	-0.26723		3.813623 1.261313		0.933973
	1.365899				2.032076
	-0.2374		1.2608	15	4.827882
	1.317172		3.8134	-51	3.730309
	-0.28542		3.8129	97	6.527409
	1.346479		1.260749		7.626908
	-1.87722		3.813776		9.292987
	-0.22316		1.263229		10.50736
	-1.89731		1.2622	.14	13.27185
	-1.21578		3.814559 3.813547		12.1669
	-2.88892				14.92997
	-1.23324		1.2629	15	16.14256
HJ-II, int3	a= 3.129	b= 5.087	c=17.713	α=90.0°	$\beta = 105.4^{\circ} \gamma = 90.0^{\circ}$
	Х		Y 3.807248 1.263052 1.262304		Z
	-0.37969				0.838837
	1.206964				2.069911
	-0.38969				4.887109
	1.157743		3.8062	.01	3.65027
	-0.42824		3.8061	18	6.469006
	1.14615		1.2624	34	7.699129
	-1.98207		3.8061	49	9.234769
	-0.40322		1.2628	803	10.64646

	-1.97566	1.263264	13.51695
	-1.95442	3.806455	12.09727
	-3.52096	3.807606	14.96936
	-1.93291	1.261953	16.38112
ts5	a= 3.147	$b = 5.047$ $c = 17.939$ $\alpha = 90.0^{\circ}$	$\beta = 107.8^{\circ} \gamma = 97.0^{\circ}$
	Х	Y	Ζ
	-0.26937	3.786473	0.828571
	1.414518	1.262492	2.13233
	-0.20074	1.26299	4.872819
	0.562624	3.786185	3.724435
	-1.05343	3.786882	6.465223
	0.629027	1.263217	7.770206
	-2.56254	3.786744	9.276017
	-0.97524	1.262959	10.67456
	-2.57641	1.263558	13.54806
	-2.56362	3.786924	12.12815
	-4.16372	3.787497	15.00199
	-2.57483	1.263523	16.39955
ω-phase	a= 3.110	b= 5.023 c= 18.146 a= 90.0°	β= 107.2° γ=90.0°
	Х	Y	Ζ
	0.028022	3.764211	0.72929
	1.663281	1.253507	2.1672
	0.243382	1.251384	5.062601
	0.186679	3.763784	3.605641
	-1.23318	3.761712	6.500877
	0.401989	1.249031	7.939045
	-2.6519	3.758874	9.396066
	-1.01699	1.246181	10.83521
	-2.43698	1.244118	13.73083
	-2.49348	3.756518	12.27314
	-3.91364	3.754386	15.1693
	-2.27876	1.243694	16.6084