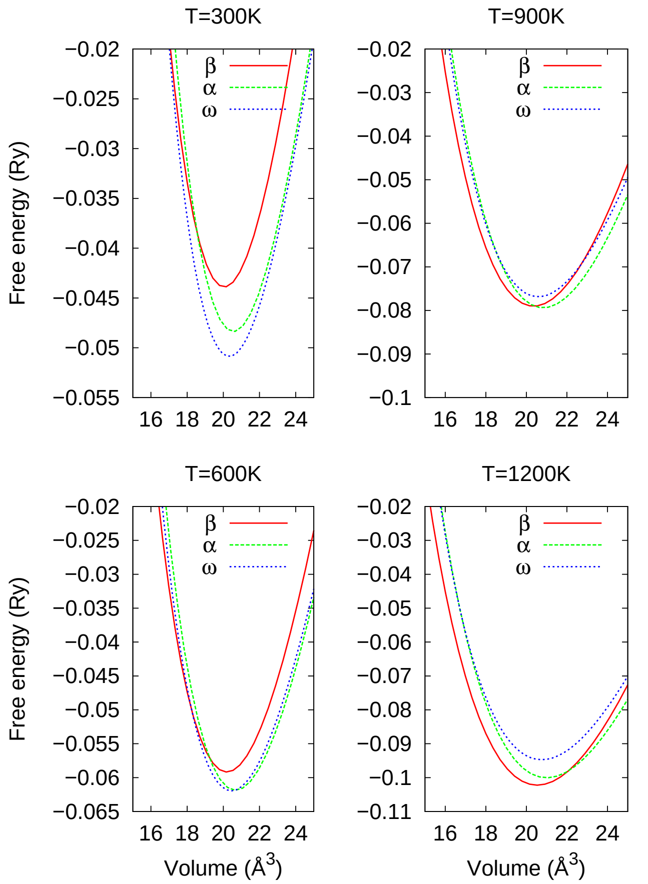

FIG. 3: Free energy of the α, ω and β phases of TiZr at different temperatures

transition at room temperature are taken from Refs.[2,3].

On the whole, a good agreement of the calculated triple point ($P_{theor} = 4.2$ GPa, $T_{theor} = 720$ K) with the experimental values $P_{exp} = 4.9 \pm 0.3$ GPa, $T_{exp} = 733 \pm 30$ K[1] is observed. At zero pressure the calculated temperature of the $\beta - \alpha$ transition is $T^{theor}_{\beta-\alpha} = 943$ K. This value is higher than the experimental one, $T^{exp}_{\beta-\alpha} = 852$ K, defined in Ref.[1] as the average of the temperatures of the transition onset on heating and cooling. It should be noted that a large hysteresis is observed upon the $\alpha - \beta$ transformation in TiZr. At atmospheric pressure the maxima of thermal peaks in the DTA curves fall on $T \sim 912$ K on heating and $T \sim 810$ K on cooling, the typical peak width being $\Delta T \sim 40$ K. With this in mind, one can consider the results of calculation of the $\alpha - \beta$ equilibrium boundary in the Debye-Grüneisen model as quite satisfactory.

The greatest discrepancy between the theoretical calculation and the experimental evidence available is observed for the $\alpha - \omega$ transition. In Ref.[3] the pressure at which this transition occurs at room temperature was estimated to be $P^{exp}_{\alpha-\omega} = 6.6$ GPa. Note thet equilibrium point of the α and ω phases was determined under shear-strain conditions at pressures up to 9 GPa. The shearing strain is known to lower the pressure at which the phase transition begins. Presumably for this reason the authors of Ref.[3] failed to obtain the $\alpha - \omega$ transition at room temperature under quasi-hydrostatic conditions. In Ref.[2] it was shown by X-ray diffraction method that the α phase of TiZr remains the sole stable phase under quasi-hydrostatic pressure up to 12.2 GPa. Only from 5.5 GPa on, becomes dominating the ω phase which remains stable up to 56.9 GPa. At pressures above 56.9 GPa there forms a high-pressure phase with a bcc lattice.

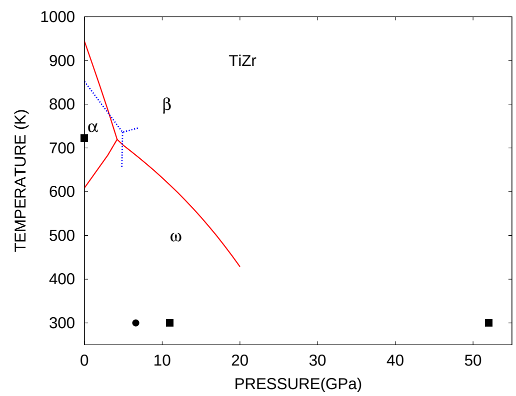

FIG. 4: The P-T phase diagram of TiZr. The solid line shows the calculation results. The dotted lines are constructed from the experimental data [1]. The experimental values for the $\alpha - \omega$ transition at room temperature are taken from Refs.: ● - [3], ■ - [2].

As seen from Fig.4, in our calculation at atmospheric pressure and low temperatures the ω phase is stable, there occurs no $\alpha - \omega$ transition at room temperature. Note that in our calculations of pure Ti[10] and Zr[11], in complete agreement with the experimental data, the α phase is stable at atmospheric pressure and room temperature, and the ω phase is stable only under pressure. That the ω phase in TiZr at normal conditions is energetically preferable, immediately follows from a comparison of the calculated free energies (see Fig.3). Recall that the difference in energy between the α and ω structures in the equiatomic TiZr alloy is almost five times greater than in pure titanium and zirconium.

The discrepancy between experiment and theory may be due to the fact that the calculation was performed for ideal crystalline structures (see Fig.1),whereas the experimental samples were imperfect crystals with lattice defects. In particular, it was shown[3] that in a TiZr alloy shear-strained under pressure the ω phase is represented by aggregations of oblong particles with characteristic size of 3$-$5 nm, and 15$-$30 nm long. If $\omega-$phase particles are situated in a coarse grain of α phase, they are mainly located at its boundaries. It was also noted[1] that various imperfect structures in samples pre-treated in different ways have a noticeable effect on the course of structural transformations. Evidently, we could not model a real