Temperature effects on structural and thermodynamic properties of $ZrAl_3$ intermetallic compound

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The structural and thermodynamic properties of the $L1_2$ structure of the $ZrAl_3$ intermetallic compound under high temperature are investigated by using *ab initio* plane-wave pseudopotential Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA).

The relative stabilities of L12, D022 and D023 structures in the ZrAl3 intermetallic compound have been widely studied [1], knowing that these theoretical calculations are carried out assuming absolute zero (0 K).

The aim of the present study is to take into account the effect of temperature to describe more realistically the structural properties of the ZrAl3 intermetallic compound.

Our first results of the formation energies show that the cubic $L1_2$ structure is metastable compared to the tetragonal $D0_{22}$ and $D0_{23}$ ones. These results are in agreement with theoretical [1] and experimental conclusions previously reported [2].The thermodynamic properties of the cubic $ZrAl_3$ structure are predicted by using the quasi-harmonic Debye model. The Debye temperature Θ, the bulk modulus B, the heat capacity Cv, and the thermal expansion α are calculated as function of temperature in the range of 0-2000K.

The effects of temperature on the structural stability of the $L1_2$ structure are discussed. The results are compared to the experimental measurements obtained from the Differential Scanning Calorimetry (DSC) showing a phase transition occurring close to 600°C.

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