

Occurrence of superconductivity in diboride of Zr

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Abstract

The contradictory reports about possible superconducting transition in ZrB_2 make it more interesting to study this system in all possible directions. The calculated elastic behaviour of the diboride of Zr is compared with the experimental values of ZrB_2 and a similar type of material TiB_2 . The analysis of calculated density of states and band structure do not indicate superconductivity in the compound.

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1. Introduction

The discovery of superconducting MgB_2 ($T_c \sim 40$ K) [1] has triggered renewed interests and impetus to actively search for novel superconductors among related compounds with the structure and chemistry similar to MgB_2 . A latest review [2] shows that diborides of transitional metals MB_2 ($M = \text{Zr}, \text{V}, \text{Ti}, \text{Cr}, \text{Mo}$) do not superconduct so far with the exception of NbB_2 . Since then several contradictory reports about supercon-

ductivity of ZrB_2 appeared. The study of Gasparov et al. [3] of temperature dependence of resistivity and ac susceptibility reveal a superconducting transition of ZrB_2 with $T_c = 5.5$ K. Pereira et al. [4] studied experimentally the pressure behaviour of ZrB_2 and VB_2 , which shows no phase transition up to a pressure of 50 GPa. Naidyuk et al. [5] investigated electron–phonon interaction (EPI) in ZrB_2 by point-contact spectroscopy. The estimated value of $\lambda \leq 0.1$ questioned the reported bulk superconductivity in this compound. Singh [6] made a theoretical study of EPI in ZrB_2 and TaB_2 . The bonding nature of transition metal diborides is analyzed via the density of states (DOS) histogram as well as the charge density plots

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by Vajeeston et al. [7]. The elastic and structural properties, DOS and band structure of ZrB_2 have been investigated in the present study. The occurrence of ‘superconductivity’ in ZrB_2 is also discussed.

2. Method of calculations

The ab initio self-consistent field (SCF) Hartree–Fock linear combination of atomic orbitals, HF-LCAO method has been used in the present investigations [8]. The electron–electron interaction was treated within the local density approximation (LDA) with the exchange–correlation functional [9]. The integrations over the Brillouin zone (BZ) are performed using the Monkhorst–Pack scheme [10]. In our present calculations, valance-electron basis sets Durand [11] and ECP HAYWSC [12] have been used for B and Zr, respectively. The exponents of the most diffuse sp and d shells for each atom have been optimized by searching for the minimum crystalline energy.

3. Results and discussion

We have determined five elastic constants, bulk modulus and the pressure derivative of bulk modulus for ZrB_2 . First the energy is calculated as a function of unit cell volume V . It is then minimized as a function of c/a ratio for the selected volume. The calculated values of $\Delta E (=E - E_0$, where E_0 is the equilibrium energy) have been plotted as a function of volume (V) in Fig. 1. The solid curve is the fitting of Murnaghan equation-of-state [13]. The inset of Fig. 1, displaying lattice param-

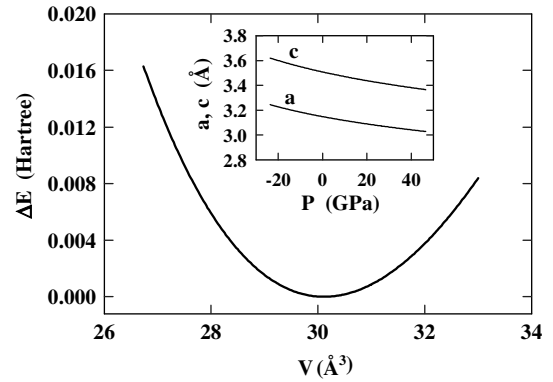


Fig. 1. The energy (ΔE) as a function of primitive cell volume (V) of ZrB_2 . The inset shows the lattice parameters as a function of pressure (P).

ters a and c as a function of pressure, shows clearly the isotropy in bonding of ZrB_2 . The calculated lattice parameters are compared with the X-ray diffraction measurement [14].

The bulk modulus B_0 at $P = 0$ and its pressure dependence, $B'_0 (=dB_0/dP)$ are also found by fitting the $E(V)$ curve (Fig. 1) by the Murnaghan equation-of-state [13]. The linear bulk modulus at $P = 0$ along the crystallographic axes a - and c - (B_{a0} and B_{c0}) and their pressure derivatives are obtained from Fig. 1 (inset) and the thermodynamic relationship, $P = -\frac{dE}{dV} = \frac{B_0}{B'_0} \left[V_n^{-B'_0} - 1 \right]$. These calculated values of bulk moduli are also presented in Table 1. Comparison with the experimental values due to Pereira et al. [4] shows that obtained values are reasonably good.

There are five independent components of the elasticity tensor for ZrB_2 . With these five distinct lattice deformations, we have calculated the energy using the appropriate expressions [15].

Table 1

Structural parameters, Bulk modulus (B_0), pressure derivative of bulk modulus (B'_0), and their in- and out-of-plane linear values for ZrB_2

Methods	a (Å)	c (Å)	V (Å ³)	B_0 (GPa)	B'_0	B_{a0} (GPa)	B'_{a0}	B_{c0} (GPa)	B'_{c0}	Ref.
LCAO-DFT	3.1832	3.5464	31.12	276	3.93	841.0	12.1	800	11.2	This
TB-LMTO	3.1970	3.5610	31.52	275	4.0 ^a	—	—	—	—	[7]
X-ray diffraction	3.1650	3.5470	30.77	—	—	—	—	—	—	[14] ^b
X-ray diffraction	—	—	—	317 ± 7	4.0 ^a	1143 ± 18	4.0 ^a	955 ± 17	4.0 ^a	[4] ^b

^a Kept fixed during fitting.

^b Experimental data.

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