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Elastic properties and phonon dispersion of bcc vanadium under pressure from first principles

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Abstract. We investigate the elastic properties and phonon dispersion of the body-centered cubic structure vanadium (V) under pressure by using the generalized gradient approximation (GGA). Our elastic constants of V at zero pressure and zero temperature are in good agreement with the available experimental data and other theoretical data. The pressure dependences of bulk modulus B and its pressure derivative B', shear modulus G, elastic Debye temperature Θ_E, elastic anisotropy factor A, Poisson ratios σ and Kleinmann parameter ζ are also presented. An analysis for the calculated elastic constants has been made to reveal the mechanical unstability of V up to 100 GPa. For the phonon dispersions of V, it is easily seen that the phonon frequencies increase as the volume decreases, the phonon mode linked to a Kohn anomaly has softened to negative values.

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Key words: vanadium; elastic properties; phonon dispersion; density functional theory

1 Introduction

Vanadium (V), one of the group-VB transition metals, crystallizes in the body-centered cubic (bcc) structure at ambient conditions. It has been attracted much more considerable attention due to its high thermal, low compressibility, and chemical stability. Up to date, many interesting on the fundamental physical and chemical properties of V have been reported in high-pressure experiments and theories [1-19].

Early in 1972, Simth [7] measured the superconducting transition temperature of V as a function of hydrostatic pressure up to 2.4 GPa and found a linear increase in T_c

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with dT_C/dP=0.062 K/GPa. Later in 2000, Ishizuka *et al.* [8] reported a superconducting transition temperature of 17.5 K at 120 GPa. In addition, Skriver [9], Moriarty [10], and Grad *et al.* [11] predicted the stability of V in the bcc structure up to at least a couple of hundred GPa. Takemura [12] proved the speculation by diamond-anvil cell experiment. However, Ding *et al.* [13] measured a phase transition of V from the bcc structure to the rhombohedral phase at 69 GPa by the diamond-anvil cell and synchrotron X-ray diffraction method. Furthermore, Jenei *et al.* [14] identified a transition pressure at 30 GPa at room temperature through nonhydrostatic compression, which is much lower than the value reported by Ding *et al.* [13].

On the other hand, several theoretical methods have been applied to investigate the properties of V. Otani and his co-worker [5, 15] investigated the lattice dynamics of V in the pressure range up to 1.5 Mbar using full-potential linear muffin-tin orbital (FP-LMTO) method. They found that the transverse acoustic phonon mode shows a dramatic softening under pressure and becomes imaginary at pressure above 130 GPa, indicating the possibility of a structural phase transition. Lee *et al.* [16, 17] declared two different rhombohedral phases which differ from each other only in the angle between the rhombohedral basis vectors. Qiu and Marcus [18] obtained three first-order phase transitions from crossings of the Gibbs free energies functions curves. With the density functional perturbation theory (DFPT), Luo *et al.* [19] obtained the phase transitions [bcc→hR1(110.5°)→distorted hR2 (108.2°)→bcc] with the increasing pressure. Landa *et al.* [5] found that the structure transition from the bcc to rhombohedral phase at 60 GPa, and then to the bcc phase again at 310 GPa.

As is known that, the phonon-dispersion relations of the bcc structure V could not be determined by conventional inelastic neutron scattering techniques since its cross section for neutron scattering is almost totally incoherent [20]. Instead, people use the thermal diffuse scattering of X-rays to measure the phonon frequencies along principle symmetry directions [15, 21, 22]. The experimental phonon dispersion curve of bcc V at ambient conditions has been measured by thermal diffuse scattering and found that for the longitudinal (111) branch it exhibits a dip near the (2/3, 2/3, 2/3) site [20-22]. However, by using the inelastic X-ray scattering (IXS), Boska *et al.* [23] revealed several phonon-dispersion anomalies clearly, whereas few theoretical methods are applied to investigate the properties of phonon dispersion.

In this work, we focus on the elastic properties and phonon dispersion of V under pressure by the plane-wave pseudopotential density functional theory (DFT) method through the Cambridge Serial Total Energy package (CASTEP) program [24, 25]. The rest of the paper is organized as follows. The theoretical method and computation details are given in Section 2. Some results and discussion are presented in Section 3. Finally, the summary of our main results are given in Section 4.