



Effect of negative pressure on superconducting transition temperature of MgB_2

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ABSTRACT

Atomistic simulation has been performed with interatomic potentials to investigate the effect of negative hydrostatic pressure on the superconducting transition temperature (T_c) of MgB_2 . The calculation reveals that T_c can be greatly enhanced by applying negative pressure and it can reach up to 52.2 K at -13 GPa, about 13 K higher than that at ambient pressure. The mechanism for the enhancement of T_c is attributed to that negative pressure reduces high-frequency phonon vibrations of B and thus dramatically enhances the electron–phonon coupling. Our result seems to open up a possible way for the enhancement of T_c in MgB_2 .

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1. Introduction

The discovery of non-copper-oxide MgB_2 , which has relatively high T_c (~ 39 K) and simple hexagonal structure, has aroused enormous interest [1]. Researchers have made great efforts to try to enhance the T_c further by employing various methods such as isotopic substitution, neutron irradiation, and chemical doping. However, Mg isotopic substitution had almost no effect on the T_c [2]. Neutron irradiation resulted in a significant reduction of T_c due to the radiation-induced disorder, although it could be healed after post high-temperature annealing [3]. For chemical doping in MgB_2 , dopants like Al, Fe and Cu were tried to substitute at the Mg site [4,5], and for B site C was the most tried dopant [6]. Nevertheless, the results found that T_c was suppressed for most of the dopants due to the formation of fine secondary phase, disorders and crystal lattice distortions. High-pressure experiments on MgB_2 have been carried out with pressure up to 40 GPa in anticipation of T_c enhancement. On the contrary, the results revealed that T_c was depressed at positive pressure [7–9]. For even higher positive pressure, density-functional-based calculation found that the superconductivity in MgB_2 vanished by 100 GPa, and then reappeared at a pressure of 137 GPa with $T_c = 2$ K [10]. However, the recent first-principles investigation demonstrated that this was not the case, instead, T_c reduced monotonically and finally vanished at 200 GPa [11]. The recent report by Ma et al. predicted a KHg_2 -type polymorph of MgB_2 above ultrahigh pressure of 190 GPa

through *ab initio* simulation, and this high-pressure phase was absent of superconductivity [12].

Up to date, most of the attempts to enhance T_c of MgB_2 give disappointing results, although there are some exceptional cases such as in strained MgB_2 films and ^{10}B isotope substituted samples. MgB_2 thin film grown epitaxially on (0 0 0 1) SiC substrate [13] or boron crystal [14] exhibited an enhanced T_c above 41 K and the T_c enhancement was attributed to tensile strain. In the case of boron isotopic substitution, T_c was increased by ~ 1 K for Mg^{10}B_2 compared to Mg^{11}B_2 [2]. Although in these samples the enhancement of T_c has been observed, the extent is quite small and only about 1–2.5 K.

Negative pressure is allowed for condensed matters and can be a few hundred MPa for liquids and a few GPa for solids [15]. Presently, modern experimental methods can generate negative pressure with a variety of techniques such as Berthelot-method and shock waves [16,17], which make it possible to investigate the substance properties at negative pressures. Researchers have studied the effect of negative pressure on structure and properties of materials such as Si [18], TiO_2 [19,20], Sb_2Te_3 [21], ice [22], and even the potato starch (biological molecules) [23] theoretically and experimentally, and found it could result in phase transition or lead to remarkable change of properties. Some researchers have also speculated that T_c may be changed by negative pressure in MgB_2 [3,24,25]. Islam et al. found negative pressure could influence the band structure and Fermi level of MgB_2 by first-principles density functional calculations [26]. In this work we investigate the effect of negative hydrostatic pressure on structure and superconductivity of MgB_2 in order to search for higher T_c . It is found that T_c can be greatly enhanced up to 52.2 K at negative pressure of -13 GPa. The mechanism of this effect is also discussed briefly.

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2. Simulation method

Free energy minimization methods can identify the crystal structure of lowest energy of a material at a given temperature and pressure by adjusting the cell volume and atomic positions until the net pressure or stress is zero. The calculation is based on the widely used shell model generalization of the Born model of a solid. Details of these techniques are available in Ref. [27]. With this model, the lattice energy E can be expressed as

$$E = \frac{1}{2} \sum_{ij} \left[\frac{q_i q_j}{r_{ij}} + V(r_{ij}) \right], \quad (1)$$

where the first item is Coulombic energy introduced by long range interactions of effective charges, the second item denotes the short range interactions. Short range interaction used in this work is represented by a Buckingham potential

$$V(r) = A \exp(-r/\rho) - Cr^{-6}, \quad (2)$$

where A , ρ , and C are fitting parameters. A , ρ is related to the hardness and size of ions, while C represents Van der waals' forces between ions. To describe the polarization of ions, shell model [28] is employed embodied in the GULP code [29], in which the interaction between the core and shell of any ion is treated as harmonic with a spring constant k and the interaction is represented by

$$E_v(d_i) = \frac{1}{2} k d_i^2, \quad (3)$$

where d_i is the relative displacement of core and shell of ion i . The polarization of a massless shell with Y charge and a core with X charge ($X + Y$ is the charge of the ion) can be calculated as

$$\alpha = \frac{Y^2}{k}, \quad (4)$$

where Y is related to dielectric constant, and k is the force constant between core and shell, related to the phonon frequency. Parameters Y and k are fitting parameters. This method has been successfully used to the simulation of colossal magnetoresistance material [30,31], $A_4B_3O_{12}$ δ -phase [32], thermal-transport properties of $SrTiO_3$ [33], surface behaviour of dolomite $CaMg(CO_3)_2$ [34], pressure effect on the properties in 410/[001] tilt grain boundary of MgO [35], $YBa_2Cu_3O_8$ [36] and MgB_2 [37].

It should be stressed that the reliability of the simulation strongly depends on the validity of the potential model used, and the latter is assessed primarily by its ability to reproduce experimental properties. All the potential parameters of MgB_2 used in this calculation, were developed in our group [37]. The difference in lattice constants and bond lengths of MgB_2 between calculated and experimental data is less than 0.0005 Å. This potential model has been used successfully for simulating the effect of positive pressure on MgB_2 up to 240 GPa. We also compared our structural data of MgB_2 under negative pressure with the available structural results from first-principles density functional calculations [26] and found that they are in good agreement (Fig. 1). This good agreement suggests that our potential can be applied to negative pressure.

3. Results and discussion

The pressure effect on lattice parameters of MgB_2 over the range from 20 GPa to -13.4 GPa was shown in Fig. 1. The lattice parameters a and c increase monotonically over the studied pressure range, and c changes more rapidly than lattice parameter a , which means that the interplane Mg–B bond is weaker than the intraplane Mg–Mg and B–B bonds. Accordingly, the c/a ratio increases almost linearly to -13.4 GPa. The calculation also reveals that

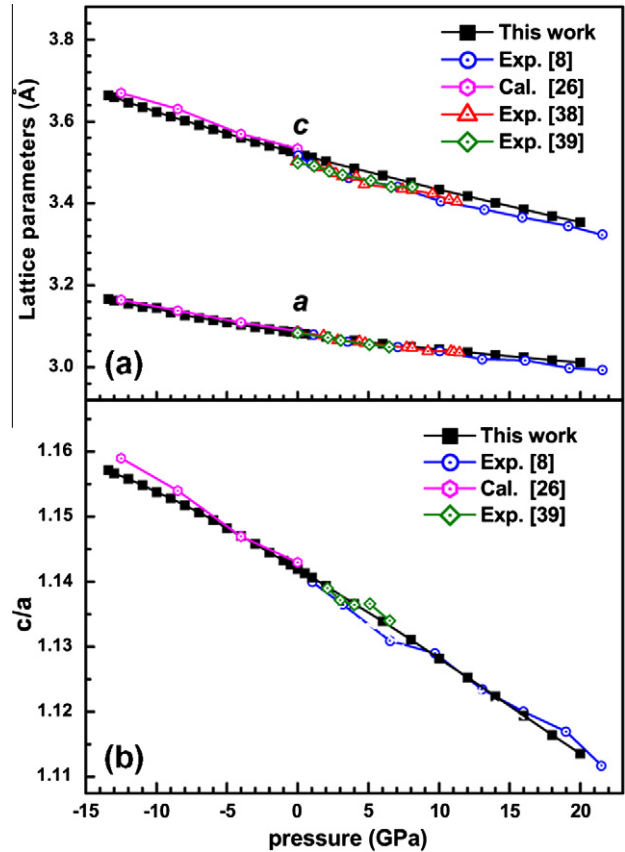


Fig. 1. Variation of calculated (Cal) lattice parameters and c/a ratio of MgB_2 with pressure compared to experimental (Exp) data.

intraplane bond angles (B–B–B and Mg–Mg–Mg) remain 120° in the studied pressure range (not shown here). Our calculated results are in excellent agreement with the experimental data at positive pressures [8,38,39] and the calculated data at negative pressures by first-principles density functional calculations [26]. This lends a support for the validity of the potential we used under both positive pressure and negative pressure.

The structural stability of MgB_2 under pressure has also been examined through lattice dynamics calculation. Fig. 2 illustrates the pressure dependence of the calculated phonon frequencies at

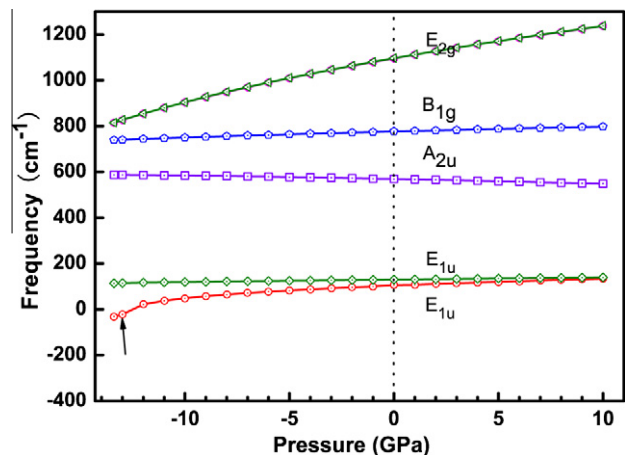


Fig. 2. Pressure dependence of the Γ -point vibrational frequencies of MgB_2 , the labeling of the modes follows Ref. [40]. Note that the E_{2g} mode is doubly degenerate.

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