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ELASTIC PROPERTIES OF LIGHT RARE-GAS CRYSTALS UNDER PRESSURE IN THE MODEL OF DEFORMABLE ATOMS

In the experimental study of the elastic properties of the material at high pressure, causing several specific problems that require theory developed specifically for given conditions. These problems include the many-body and quadrupole interactions in lattice dynamics.

In this work, we construct the nonempirical version of the model of lattice dynamics with deformable atoms, which was developed by K.B. Tolpygo for rare-gas crystals. This model, within a unified approach, allows one to obtain both the short-range three-body interaction and the quadrupole interaction associated with the quadrupole-type deformation of electron shells of the atoms during the displacements of the nuclei.

Low energy of interatomic interaction of closed spherically symmetric shells results in the fact that atoms weakly deform each other. But this effect does not give grounds to ignore this deformation because only it is responsible for the bond of atoms in a crystal as seen by the example of Van der Waals forces.

On the basis of nonempirical version of Tolpygo model the quantitative analysis within the framework of core and deformed shell model allowed to ground a model and approaching for the calculation of many-body interaction at description of elastic properties in area of metallization region of Ne and Ar. Three-body interaction is specified due to the account in parameters of holdings of all overlap integrals of external *p*-orbitals. Research of conduct of holdings of three-body and quadrupole interactions in the Birch elastic moduli and deviation from Cauchy relation δ are conducted in the wide pressure range. Many-body interaction prevails in the case of Ar, and for compressed Ar deviation from Cauchy relation is negative, the value of which is increase with growth of pressure. Contributions from many-body and quadrupole interactions in Ne with good exactness are compensated, that provides for δ a positive value poorly depending on pressure. Agreement with the experiment of the calculated elastic moduli and deviation from Cauchy relation are good.

The present *ab initio* research of the Cauchy relation violation gave us an opportunity to recognize the nature and the correlation of forces which form the elastic properties of crystals under high pressures. The Cauchy relation violation in rare-gas crystals is conditioned with two reasons: firstly – with the three-body forces which are induced by the atom electron shells' overlapping in the crystal; secondly – with the quadrupole interaction related to the atom electron shells' deformation of the quadrupole type at the nuclei displacement.

Keywords: rare-gas crystals, deformation of electron shells, quadrupole interaction, many-body interaction, high pressure, short-range repulsion, overlap integral, Cauchy relation

Fig. 1. Interatomic distance R dependence of overlap integrals of the nearest neighbor orbitals: *1* – $2p_z2p_z$ and *2* – $2p_x2p_x$ for Ar; *3* – $2p_z2p_z$ and *4* – $2p_x2p_x$ for Ne

Fig. 2. Pressure dependence of Birch elastic moduli B_{ij}: *а* – for Ne; *б* – for Ar; --■-- – the present calculation of B_{11}^0 [23]; –■– – the present calculation of B_{11} allowing for contri-

butions of three-body and quadrupole interactions $B_{11} = B_{11}^{0} + B_{11}^{t} + B_{11}^{q}$; □ – the experiment [14,12]; --◓--, –●–, ○ and --◬--, –▲–, △ – the same for B_{12} and B_{44}, respectively

Fig. 3. Pressure dependence of Birch elastic modulus B_{12} for Ne: --◓-- – B_{12}^{0} calculation in M3-model [23]; –■– – calculation taking into account three-body interaction and quadrupole interaction $B_{12} = B_{12}^{0} + B_{12}^{t} + B_{12}^{q}$ at $S = S_{zz} + S_{xx}$; ···· – the same at $S = S_{zz}$; ··◇·· – calculation in DFT [24]; –·– – calculation in many-body model EAM with empiric potentials [25]. The arrow indicates the calculated value of compression metallization [8]

Fig. 4. Pressure dependence of deviation from Cauchy relation δ (10) for Ne (*a*) and Ar (*б*): –■– – the present calculation $\delta = \delta_t + \delta_q$ at $V_q^0 = V_q^{\exp}$, $A = 0.5$ (for Ne) and $A = 0.1$ (for Ar) (see (24) in [18]); –●– – the same at $V_q^0 = |V_t|$, $A = 1$ for Ne; –□– – the present calculation taking into account three-body interaction δ_t ($V_q = T = 0$); – – – calculation in DFT [24]; –·– – calculation in many-body model with empiric potentials [25]; ☆ – the experiment [13]