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QUADRUPOLE INTERACTION IN LATTICE DYNAMICS OF COMPRESSED RARE-GAS CRYSTALS IN A MODEL OF DEFORMABLE ATOMS. 3. ELASTIC PROPERTIES AND THE CAUCHY RELATIONS FOR Kr AND Xe

The study of atomic properties of crystals at the increasing pressures has been of great interest, since the end of the last century, due to the opportunities in the experimental technique. The study of the elastic properties of compressed rare-gas crystals is of particular interest because they are widely used as pressure media in the experimental facilities, being convenient objects for the development and debugging of new calculation methods.

In this work, we developed the quantum mechanical model of deformable and polarizable atoms (the model by K.B. Tolpygo) for the research of the elastic properties of rare-gas crystals of Kr and Xe in a wide range of pressure. It is shown that it is impossible to reproduce the observed deviation from the Cauchy relation $\delta(p)$ for Kr and Xe adequately with taking into account the many-body interaction only. The individual dependence $\delta(p)$ for each of the crystals is the result of two competing interactions, the many-body interaction and the quadrupole interaction one generated by the deformation of atoms' electron shells when nuclei are displaced. Contributions of these interactions to Kr and Xe compensate each other with high precision that provides δ with a value which is weakly dependent on pressure. This result is in a good agreement with the experimental data in contrast to *ab initio* calculations in the density functional theory.

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

Fig. 1. The compression dependence of the three-body parameter V_t and the quadrupole parameter V_q at different coefficients A_i for Kr (*a*) and Xe (*б*): ▲, ●, ■ – calculated quadrupole parameters V_q with the coefficients A_i = 0.6, 0.5, 0.4 (12) respectively; □ – three-body parameter V_t (6); ☆ – V_q calculated by formula (13) at $\delta = \delta_{\text{exp}}$ [10]

Fig. 2. Pressure dependences of the Birch elastic moduli B_{ij} (*a*), B_{12} (*б*), B_{44} (*в*) for Kr: - -■- - – calculations of $B_{11}^0(M3)$ in the M3 model [41]; ■ – the present calculation of B_{11} allowing for contributions of three-body and quadrupole interactions $B_{11} = B_{11}^0 + B_{11}^t + B_{11}^q$; □ – the experiment [11]; ◓, ●, ○ and - -▲- -, ▲, △ – the same for B_{12} and B_{44} respectively; ··· – calculations of $B_{12}^0(M1)$ in the M1 model; –··– – calculation of B_{12} in the model M1 with B_{12}^t and B_{12}^q taken into account; –·– – calculation in EAM [2], —✩— – calculation in DFT [1]. The calculated value of metallization pressure p_m = 310 GPa is marked with the arrow [46]

Fig. 3. Pressure dependences of the Birch elastic moduli B_{ij} (*a*), B_{12} (*б*), B_{44} (*в*) for Xe. The experiment was taken from [10]. The average value of metallization pressure p_m from 121 to 138 GPa is marked by the arrow [47,48]. The other notations are as in Fig. 2

Fig. 4. Pressure dependences of the deviations from the Cauchy relation $\delta(p)$ for Kr (*a*) and Xe (*б*): ▲, ●, ■ – the present calculations $\delta = \delta_t + \delta_q$ at $V_q^0 = V_{\exp}^0$, A_i = 0.6, 0.5, 0.4 respectively; □ – calculation with account of three-body interaction only $\delta_q = 0$; –·– – calculation in EAM [2]; –○– – calculation in DFT [1]; ☆ – the experiment [11]