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LOW-*Z* MATERIALS BEHAVIOR AT HIGH PRESSURES

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Pressure dependence of band structure of solid neon is investigated ab-initio. Bandwidth and band energies are enhanced as the pressure is increased up to $\Delta V/V_0 = 0.7$. *Further, harsh drop of the lowest conduction band-energy is seen in the Brillouin zone faces centers. It causes a metallization at the compression ratio* $\Delta V/V_0 = 0.78 \pm 0.01$; $p_m = 3.5 \pm 0.7$ *Mbar.*

When the pressure reaches megabar, values pressure-induced energy change in a crystal becomes comparable with its cohesive energy. Crucial modification of chemical bond type takes place in a crystal, namely, insulator-metal transition or metallization which is defined as forbidden gap closure in energy spectrum of insulator. One takes moderate interest in the materials with low atomic number (low-*Z* materials) since these substances possess high compressibility, with the pressure effects being essential. Rare gas crystal neon is one of the low-*Z* materials. Moreover, investigating the properties and the metallization of compressed rare gas crystals is a deal of special interest because rare gases are widely used as a media able to create almost perfect hydrostatic conditions in experiment.

Ab-initio band structure calculation of solid neon at megabar pressures is presented in this paper. Occupied bands are calculated as it is proposed in [1] in the Hartree–Fock approximation using the basis of atomic orbitals orthogonalized exactly at different sites of a crystals. Then, the Abarenkov–Antonova cluster expansion (CE) [2] is applied in [3] to calculate orthogonalizing matrix. To obtain the conduction bands of compressed crystal, orthogonalized plane waves (OPW) method is modified by using occupied band wave functions calculated with the CE [3,4]. Using the CE is equivalent to taking account for all the powers in overlap integrals S of neighbour atoms orbitals. It allows one to use no small parameters like the overlap integrals which constrain the applicability of used methods by low pressures only. Moreover, two-particle cluster approximation is estimated to be applicable for compressed neon up to metallization point. All further calculations are performed in this approximation.

In Fig. 1, the band structure of solid neon is given. Conduction bands $E_{\mathbf{k}c}$ and upper $2p$- and $2s$-occupied bands $E_{\mathbf{k}v}$ are plotted. We can see an ordinary picture of insulator for uncompressed crystal. As compression is enhanced, the occupied bands are widening and rising up on the energy scale. The valence electron effective mass m^* decreases and some branches have $m^* \sim 1$ near the metallization (at the compression ratio $\Delta V/V_0 = 0.77$). Direct band gap between the energies in the Γ Brillouin zone

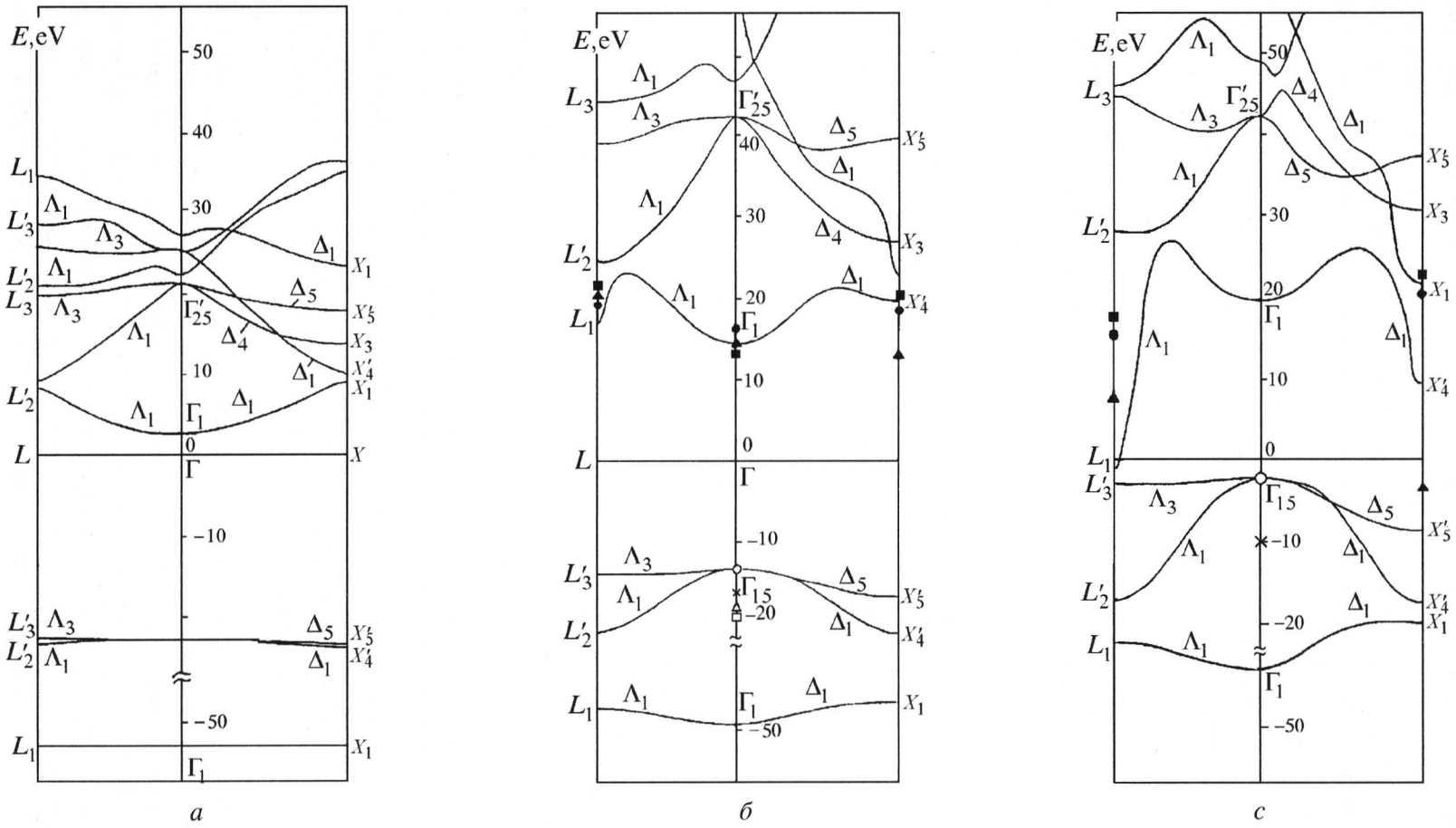

Fig. 1. Band structure of solid neon: $a - u = \Delta V/V_0 = 0$; $b - u = 0.7$; $c - u = 0.77$. Solid lines – calculation with taking all the powers in overlap integrals S into account (model 3). Full symbols – the lowest conduction band energies: ■ – standard OPW method with $S = 0$; ▲ – OPW method with orthogonalization in the first order in S

(BZ) point increases as the pressure is moderated. Indirect gaps between the top of occupied band in the Γ point and the conduction-band energies in the X and L BZ points increase too (up to $\Delta V/V_0 = 0.7$). Then, the energy of the lowest conduction band begins to drop harshly at the X and L points while all the rest energies enhance. Finally, the lowest conduction band overlaps with the upper occupied band. It causes indirect gaps closure, i.e. metallization.

In Fig. 2, the upper occupied bandwidth of neon is plotted as a function of the compression ratio $\Delta V/V_0$. The result of the Hartree–Fock method with taking all the orders in S into account is denoted by curve *3*.

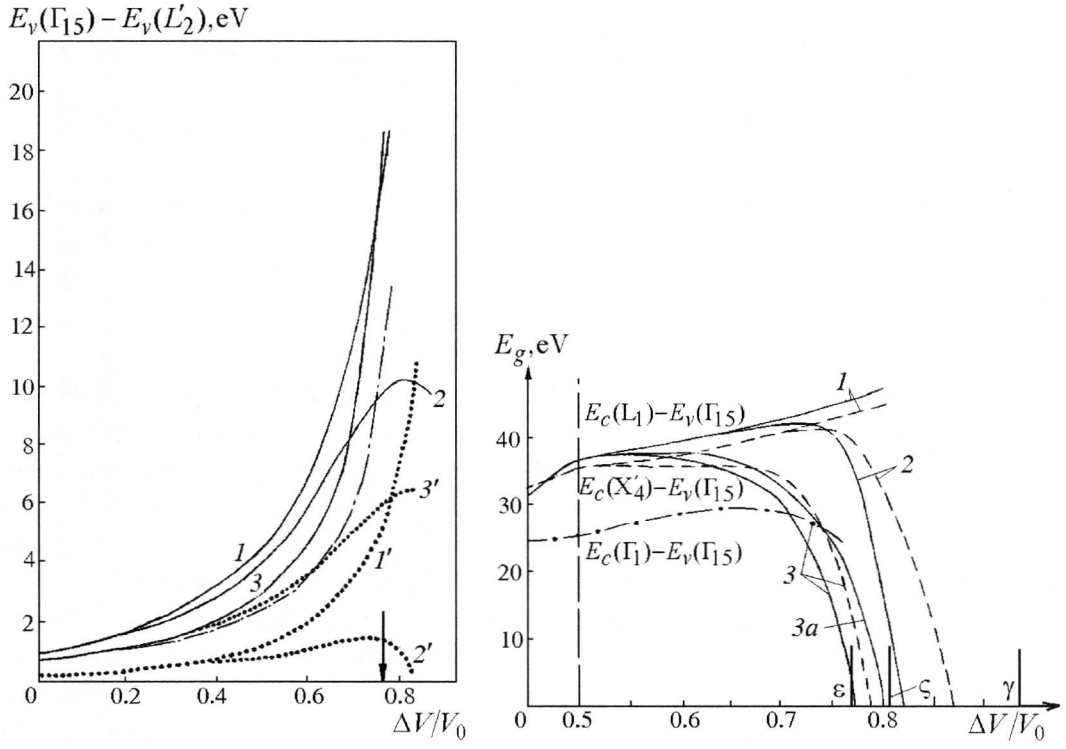

Fig. 2. Upper 2*p*-occupied bandwidth of neon. Notation of curves is the same as that of the models. Vertical arrow denotes the calculated (model 3) metallization compression

Fig. 3. Band gaps of solid neon. Indirect gaps are solid lines and dashed lines. Direct gap is dashed-dotted line. The models are denoted by the digits: *1* – $S = 0$; *2* – orthogonalization in the first order in S; *3* – accounting for all the powers in S. Vertical short lines denote calculated metallization compression: γ – [6], ε – [7], ζ – [8]

Occupied bands of solid neon are also calculated by a number of one-electron methods: standard method of linear combination of atomic orbitals (LCAO, model 1′) with $S = 0$, and its modification, cluster expansion localized orbitals method (CELO, model 2′) [3]. In the both methods the electron spectrum is determined as an energy of electron in non-self-consistent one-electron potential constructed as a sum of isolated atoms potentials. It is seen that the results of all the models listed are in agreement with each other at $\Delta V/V_0 \leq 0.4$ only, with no orthogonalization being required.

Fig. 3 shows the neon band gaps behavior via the $u = \Delta V/V_0$. One can see no band gap closure in the model which takes no overlap integrals into account (standard OPW method, curve *1*). The metallization is predicted at $u_m = 0.78 \pm 0.01$ when all the powers in S are taken into account, with the metallization pressure $p_m = 3.5 \pm$ $\pm$ 0.7 Mbar according to the equation of state calculated in [5] with the CE. Average value among all the models is $u_m = 0.80 \pm 0.03$ with the pressure spread $2.9 \leq p_m \leq 10.5$ Mbar. However, the pressure spread obtained is not so large as to give anomalous values $p_m \sim 1300$ Mbar from [6]. All our models and a number of estimations [7,8] give u_m of about 0.8, with pressure $p_m \leq 10$ Mbar.

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СТРУКТУРА И СВОЙСТВА ДИОКСИДЦИРКОНИЕВОЙ КЕРАМИКИ ИЗ НАНОПОРОШКОВ, КОМПАКТИРУЕМЫХ ВЫСОКИМ ДАВЛЕНИЕМ

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Представлены результаты исследований структуры и механических свойств оксидной керамики, которая изготавливалась из нанопорошков состава ZrO_2–3 mol.% Y_2O_3 прессованием в условиях высокого гидростатического давления в диапазоне 100–1000 МРа и спеканием при 1300–1600°С. Порошки готовились по разработанной в ДонФТИ НАНУ технологии, базирующейся на методе совместного осаждения с использованием активных физических воздействий (ультразвуковой (УЗО) и микроволновой (МВО) обработки, импульсного магнитного поля) в процессах синтеза стабилизированного иттрием диоксида циркония.