techniques). Analytic representations of the *atomic interaction lines* may be evaluated and the associated *bond path* lengths determined. The fourth section of TOPOND computes atomic properties which may be obtained either following an indirect[3] determination of the zero-flux surfaces or using a combination of the indirect with the standard[5] direct methods. The last section performs the grid evaluation of ρ, $\nabla^2\rho$, $|\nabla\rho|$ functions and traces out molecular graphs, or generically, $\nabla\rho$ trajectories in selected crystalline planes. The electron localization function (ELF), along with other local and integral properties (kinetic energy densities) which depend on the non-diagonal elements of the first order density matrix, can now also be computed.

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PS21.02.08 A TOPOLOGICAL ANALYSIS OF CHARGE DENSITIES OF THE DIAMOND, SILICON AND GERMANIUM CRYSTALS. Yu. A. Abramov, National Institute for Research in Inorganic Materials, Namiki 1-1, Tsukuba, Ibaraki 305, Japan*. *address for correspondence: Physics Department, Mendeleev University of Chemical Technology, Miusskaya Sq.9, Moscow 125047, Russia

The Hansen-Coppens multipole model of charge density has been fitted to published [1,2] highly accurate experimental and theoretical structure factors for diamond, silicon and germanium crystals. Careful consideration was given to the choice of variable parameters and to their significance. Analysis of both model experimental and model theoretical charge densities has been performed in terms of Bader's topological theory using the obtained model parameters. The general topology of the charge density appeared to be identical for all crystals, displaying the four possible types of critical points of rank three and showing no non-nuclei atractors between nearest-neighbour atoms. Properties of the charge density at the bond critical points (3,-1) and of the Laplacian distribution reflect the strong covalent bond in diamond crystal and its dramatic weakening on descending that series of crystals. This correlates with the change in semiconducting behaviour and increase in atomic displacement amplitudes at room temperature. Values of the Laplacian of charge density at the cage critical points, (3,+3), exhibit the same trend as those of the bulk modulus B.

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