DETERMINATION OF THE BASE PARAMETERS OF SEMICONDUCTOR CUBIC CRYSTALS VIA THE LATTICE CONSTANT

V.G. Litovchenko

V. Lashkarev Institute of Semiconductor Physics,
Nat. Acad. Sci. of Ukraine
(*45, Prospekt Nauky, Kyiv 03028, Ukraine;*
e-mail: LVG@isp.kiev.ua)

S u m m a r y

Similarly to the Periodic Table of Elements (PTE), a method for the characterization of the principal parameters of diamond-like crystals, which is based on the single-valued function of the lattice constant L, is proposed. Using this approach, the dependences of basic crystal parameters, such as the forbidden gap energy E_g, coefficients of covalency, metallicity, and ionicity, melting temperature, T_m, microhardness, H, and electron affinity, X_{opt}, on the lattice constant has been proposed in the form of a monotonous exponential function, $F_n(L)$. The value of L can be calculated using the well-known values of the valence radii of elements, r_A, r_B (or the distances between the neighboring atoms, A and B, in a crystal) according to the formulas: $L = \frac{2}{\sqrt{3}} r_{AB}$, $r_{AB} = (r_A + r_B)$. The obtained dependences of the crystal parameters on L open the way to predict the crystal parameters of a number of new materials such as superhard nitrogen-borocarbon (BN_2C), nitrocarbon (C_3N_4), diamond-like nanohydrocarbon ($CH_x(sp^3/sp^2)$), etc., as well as narrow-gap multicomponent semiconductors such as SiGePb(Sn) and new nanosized materials.