

Molecular Design of New Low- k Insulating Materials for Microelectronic Applications

Helmut Hermann^{1*}, Kostyantyn Zagorodniy¹, Manfred Taut¹, Gotthard Seifert²

¹Institute for Solid State and Materials Research, IFW Dresden, P.O.B. 270116, D-01171 Dresden, Germany, ²Institute of Physical Chemistry and Electrochemistry, TU Dresden Mommsenstr. 13, D-01062 Dresden, Germany

The interconnect delay time and the power dissipation appear currently as a limiting factor of the improvement of the performance of microelectronic devices. Both properties are determined by the geometrical distribution of metallic wiring and insulating layers, especially by the smallest linear dimension of the metallization system.

The delay time and the power dissipation can be diminished by introducing insulating materials with reduced dielectric constant k . While for the traditional material silicon dioxide the dielectric constant is about 4, the production of high-performance circuits will require insulating materials with k -values near or below 2 in near future.

Here we present results of computational studies of hypothetical ultralow- k insulating materials designed as covalent networks which are made up of C₆₀ fullerenes and quasi-linear molecular groups. The fullerenes act as nodes of the network whereas the quasi-linear groups form the edges. The case of a regular network with simple cubic arrangement of the fullerenes is considered in detail. In this study the quasi-linear molecular groups are realized as C_{*n*}X_{2*n*} chains with X = H, F. The structure of the systems is optimized using either the conjugate gradient or the steepest descent method at the density-functional tight-binding level [1] where periodic boundary conditions are applied. Elastic constants are determined by calculating the variation of the energy of the system due to virtual deformation. For the calculation of the dielectric constant the Clausius-Mossotti model is used as continuum theoretical approach to the interaction of a molecule and its polarizable environment [2]. Some aspects related to the conditions of applicability of this model to the type of structures considered are discussed in [3]. Results of the present computational study are shown in the following Table.

| Molecular unit | C ₆₀ (C ₂ H ₄) ₃ | C ₆₀ C ₂ F ₄ (C ₂ H ₄) ₂ | C ₆₀ (C ₂ F ₄) ₃ |
|----------------------------|---|---|---|
| <i>Dielectric constant</i> | 2.18 | 2.16 | 2.11 |
| <i>Bulk moduls, GPa</i> | 5.0 | 5.1 | 6.1 |

[1] D. Porezag, Th. Frauenheim, Th. Köhler, G. Seifert and R. Kaschner, Phys. Rev. B 51, 12947 (1995).

[2] C. J. F. Böttcher, Theory of polarization, Elsevier, Amsterdam (1973).

[3] K. Zagorodniy, M. Taut, H. Hermann, Phys. Rev. A 73, 054501 (2006).

* E-mail: h.hermann@ifw-dresden.de