

**MOLECULAR POLARIZABILITY OF Si/Ge/GaAs
CLUSTERS AND NANOSTRUCTURES**

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The role of size in modifying the properties of a material has not been exploited until recently. Based on interatomic potentials, the structure of some clusters is special. Nanocrystalline powders can be used to synthesize materials with physical processing such as sintering. In previous papers, fullerenes, Sc clusters, Sc-cluster endohedral fullerenes, graphite models and Sc hexagonal close packing were studied. In this work, the geometries of Si_n , Ge_n ($n \leq 10$) and Ga_nAs_m ($n, m \leq 4$) clusters are optimized with MMID. Polarizability measurements have recently been performed for small semiconductor clusters. Program PAPID is used for the calculation of the dipole-dipole polarizability $\bar{\alpha}$, with the interacting-induced-dipoles polarization model that calculates tensor effective anisotropic point polarizabilities by the method of Applequist *et al.* A version of PAPID has been implemented in the molecular mechanics (MM2) program and in the empirical conformational energy program for peptides (ECEPP2). The new versions are called MMID and ECEPPID. PAPID is applied to Si_n , Ge_n ($n \leq 10$) and Ga_nAs_m ($n, m \leq 4$) small clusters. The variation of the computed values for polarizability with the number of atoms is calculated. Notice that the results for Si_6 , Ge_6 , Ge_8 , Ge_9 , $GaAs_2$, Ga_2As , Ga_2As_2 , Ga_3As_4 and Ga_4As_3 are superposed. On varying the number of atoms, the clusters show numbers indicative of particularly polarizable structures. The results for the polarizability are in agreement with reference calculations from Chelikowsky carried out within the density functional theory. As a reference, the bulk limit for the polarizability is included, estimated from the Clausius-Mossotti relationship:

$$\alpha = \frac{3(\epsilon - 1)v}{4\pi(\epsilon + 2)}$$

where v is an elementary volume per atom in the crystalline state and ϵ is the bulk dielectric constant. α is taken as 3.75 \AA^3 (Si), 4.50 \AA^3 (Ge) and 4.15 \AA^3 (GaAs) per atom. The polarizability trend for these clusters as a function of size is different from what one might have expected. The clusters are all more polarizable than what one might have inferred from the bulk polarizability. Previous experimental work yielded the opposite trend for somewhat larger clusters, *i.e.*, in this work the polarizability of clusters tend to be lower than the bulk limit and approach this limit from below. At present, the origin of this difference is problematic. One might argue that smaller clusters need not behave like those of intermediate size. The high polarizability of small clusters is attributed to arise from dangling bonds at the surface of the cluster. Indeed, most of the atoms within small clusters reside on the surface. In this respect, semiconductor clusters resemble *metallic* clusters. They tend to have higher coordination numbers than those in the crystalline state. In fact, these structures are

thought to be more closely related to the high-pressure metallic phases than to the diamond structure.

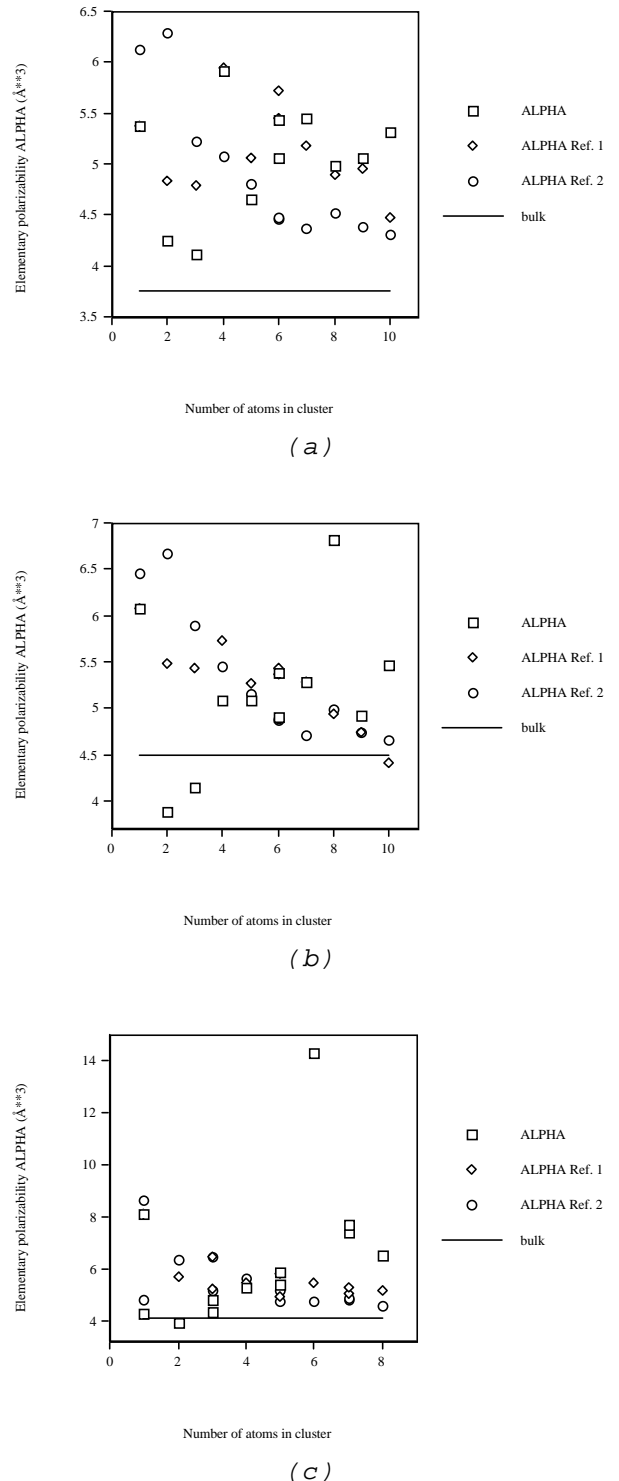


Fig. 1. Elementary polarizability of (a) Sc_n , (b) Ge_n and (c) Ga_nAs_m clusters vs. cluster size.