SELF-ORGANIZATION AND SIZE EFFECTS IN AMORPHOUS SILICON

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Abstract. *Self-organization and size effects in amorphous silicon have been investigated by modelling of the structure at nanoscale. The size effect related to the disorder in silicon is treated by the free energy balance in nanometric clusters using valence force field theory.The computed structural and energetical parameters of three continuous random network (CRN) models of amorphous silicon with 2052, 156 and 155 atoms are compared with the experimental values.In order to show the importance of the interfaces between different a-Si clusters, two networks of 200 and 205 atoms were modelled separately and then linked using an amorphous and a crystalline interface.Also the voids in the a-Si clusters are investigated.*

Keywords: size effects, amorphous silicon, nanometric clusters

I. Introduction

Extended research is dedicated for creating highly structured nanomaterials. One key issue is to form discrete organized nanoparticle aggregates, as opposed to extended homogeneous arrays [1, 2]. These discrete aggregates allow getting three-dimensional structures with diverse magnetic, electronic, and optical properties. Moreover, these assemblies could be placed on the surfaces to create devices and sensors in the 2-40 nm range. A "mortar" with recognition element-functionalized polymers is used to assemble complementary nanoparticle "bricks" [3]. Other alternative is to trigger the formation of specific aggregates or atomic configurations in rather homogeneous matrices using the energy controlled self-assembling processes. The formation of discrete regular atomic scale particles of controlled size and shape and spatial arrangement is an important step on the way to controlled nanoparticle assembly.

Amorphous, glassy and, in general, disordered materials are governed by laws not completely understood till now. The metastable configuration of the atoms gives to material the possibility to choose one among various pathways to change its free energy when, by providing some energy, the system is

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