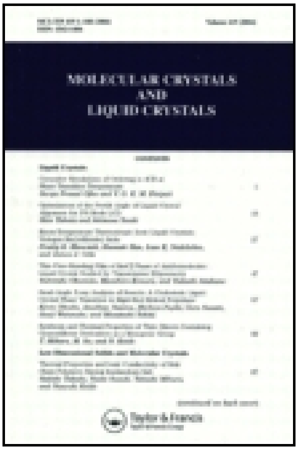

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Numerical Investigations of the Interaction of Copper Phthalocyanine Molecules with Silicon Surface

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Numerical Investigations of the Interaction of Copper Phthalocyanine Molecules with Silicon Surface

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The theoretical investigation of the scattering of copper phthalocyanine molecules in the surface field taking account of the vibration-rotational interaction was performed by molecular dynamics method, its propagator modification of the second order of accuracy. A software complex was developed to simulate the interaction of gas molecule assembly with a solid surface at a given temperature and gas volume density. Comparative analysis of molecule scattering was performed for the continuous and crystal silicon substrate models. The following elementary processes were investigated: 1) the scattering of a molecule on Si surface; 2) the collision of two molecules in gas phase; 3) the collision of two molecules one of which is bound on the Si surface.

Keywords: phthalocyanine film; molecular dynamics

INTRODUCTION

Many experimental investigations have been reported on the growth of vacuum–deposited films of various phthalocyanines[1,2], however, theoretical and numerical investigations of this phenomenon are very rare. In this paper, the theoretical investigation of the scattering of copper phthalocyanine molecules (CuPc) in the surface field taking account of the vibration-rotational interaction was performed by means of molecular dynamics method, its propagator modification of the second order of accuracy.

EXPERIMENTAL

The calculations of the vibrational spectrum of CuPc were performed within the valence force field approximation using the programme for the calculation of vibrational spectra LEV by Gribov L.A. et al.[3]. Structural parameters used are based on the results of the crystallographic analysis of β-CuPc[4] but are modified slightly to keep D_{4h} symmetry.

RESULTS AND DISCUSSION

In order to describe the behavior of the assembly of copper phthalocyanine molecules in the surface field of the silicon substrate, in the general case we consider M molecules, each of them containing 57 atoms. Intramolecular interaction is described by the sum of pair and multiparticle potentials with the constants determined when calculating the vibration spectrum. Atom-atomic approximation with the parameters determined in Ref.[5] was used to describe intermolecular interaction and the interaction of molecules with the substrate. Silicon substrate was modelled in several manners. In the most general case, a rectangular parallelepiped that containing $n_x n_y n_z$ crystal cells of silicon was considered. The interaction between silicon atoms were described by the potential suggested in Ref.[6].

The simulation of the interaction of copper phthalocyanine molecules with the silicon surface is based on the algebraic modification of classical mechanics[7]. Propagator description of the dynamics of mechanical systems of many particles and numerical schemes were tested with several problems[8, 9]. In order to simulate the potential energy of intramolecular interaction in copper phthalocyanine, force constants were calculated. For this purpose, the normal coordinate analysis for vibrations of copper phthalocyanines was carried out. The polarization measurements of oriented single crystal of copper phthalocyanine were made to determine the symmetry types of Raman modes. The isotopic frequency shifts upon ^{15}N substitution for nitrogen atoms in CuPc were measured in order to confirm the calculation. All these operations and the final variant of force field are described in detail in Ref.[10].

The adsorption of phthalocyanine molecules on silicon surface was studied within a wide range of molecule mass center velocities (10 m/s$\leq V_c \leq$600 m/s) for various angles of molecule plane relative to the substrate surface $0<\alpha<\pi/2$. The velocity vector was perpendicular to the surface. Initial temperatures of the crystal and molecule were equal to zero. Numerical analysis has shown that in the absence of rotation the molecules are adsorbed by the surface in the whole range of velocities V_c and angles α. Similar calculations were performed for the molecules with rotation. It was observed that for the frequencies above 10^{+12} s^{-1} the molecules are not adsorbed by the surface within the whole range of mass center velocities. This allows us to come to the most important practical conclusion: it is necessary to decrease the rotation energy of molecules in order to increase adsorption coefficient.

Numerical investigation of the collision of two molecules without rotation was performed within the same range of mass center velocities. Initial temperatures of the crystal and molecule were equal to zero. The planes of molecules were parallel. It was shown that the molecules form a stable cluster for the whole velocity range of interest for technological applications.

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