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ON THE THERMAL STABILITY AND MELTING TEMPERATURE OF NANO-SYSTEMS

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Various material properties which are well defined and clearly fixed for macroscopic systems, get a modified significance in nano-physics and nano-technology. It is shown, as an example, that the temperature behaviour of material systems is considerably changed when we go from macroscopic to nanometersize. It is pointed out that the standard model of solid state physics (ordered structure, harmonic approximation) is in general not sufficient for the description of nano-systems.

Keywords: molecular dynamics, thermal behaviour, material properties
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I. INTRODUCTION

Only a few years ago materials research had mainly to do with macroscopic systems. The situation changed fundamentally with the rise of nanotechnology, and this technology will have an essential influence on the development of materials research.

Properties which are well defined and clearly fixed in connection with macroscopic systems (bulk systems) are very often no longer well defined in nanophysics and nano-technology.

For example, the melting temperature and the thermal stability of nano-systems belong to those properties which can be strongly changed when we go from the macroscopic to the microscopic realm, in which we have to take into consideration the nanometer-scale properties.

II. THERMAL STABILITY OF NANO-SYSTEMS

The melting temperature of a macroscopic system is usually well defined, and the system is thermally stable up to the melting point; there can of course be phase transitions but the various phases define stable configurations.

In contrast to macroscopic systems, the melting temperature of a nano-system is dependent on the particle number and is also a function of the shape of the system. As is demonstarted in this paper, the melting temperature of certain nano-systems is not defined and not clearly fixed. This is a completely new situation, in particular in connection with materials research.

Let us demonstrate this point by means of an example. The melting temperature of aluminum is 933 K and the microscopic structure and the outer shape of macroscopic Al-systems are stable up to 933 K. That is not the case for Al-systems of nanometer-size. We did molecular dynamics calculations on the basis of a realistic pair potential[1,2], and the following results should be of particular interest:

The *thermal stability* of nano-structures sitting on the bulk surface–for example, the three-dimensional structure shown in Fig.1–will in general only be little correlated with the melting temperature. The structures are in general unstable, or will even dissolve before reaching the melting point.

In Fig.1(a) three-dimensional structure consisting of aluminum atoms is shown. As can be recognized from Fig.1(d), this Al-configuration is structurally clearly disturbed already at T =270 K, that is, far below the melting temperature. This system develops as follows: Fig.1(a) represents the configuration at the beginning of the calculation, corresponding to the structure at zero temperature. The time step used in the calculations was 5×10^{-15} s; the particle number of the nano-system is N =1660 (without substrate).

After 2000 time steps the system has a temperature of 250 K (Fig.1(b)). After 6000 time steps (Fig.1(c)) the temperature is 270 K and the system remains at this temperature hereafter, but there are still changes going on in connection with the shape of the system. After 10^4 time steps the outer form tends to be stable, as shown by Fig.1(d).

It is typical for the behaviour of such systems that

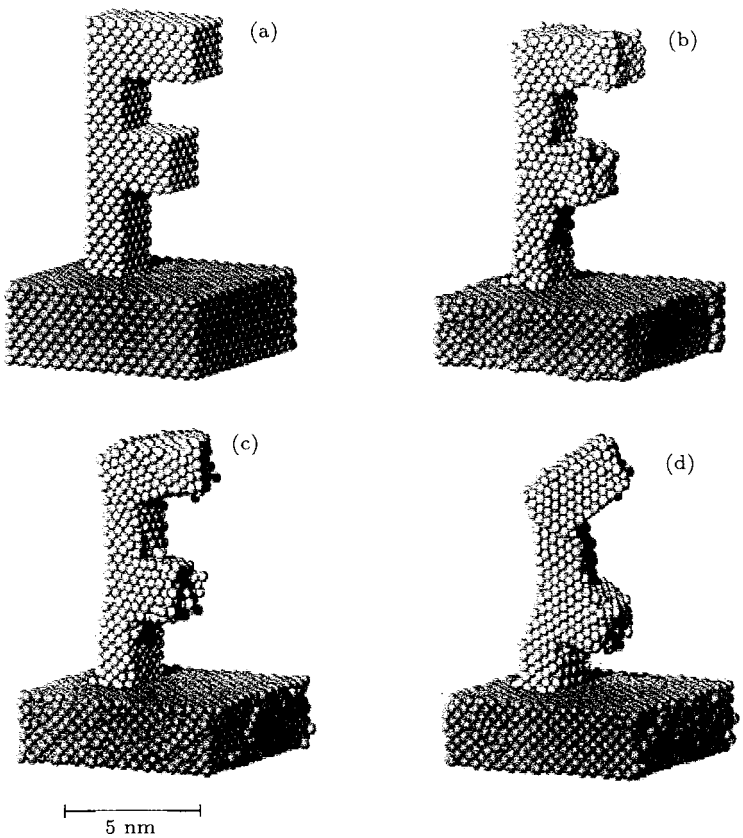


Fig.1. A molecular dynamics study of a nano-system which is positioned on a substrate; its particle number is $N = 1660$. Both the nano-structure and the substrate consist of Al atoms.

a slight variation of the initial conditions leads in general to different final shapes of the system; examples are given in Fig.2 and Fig.3.

In connection with the case studied in Fig.1, Fig.2 and Fig.3 the following is essential: The thermal behaviour is not entirely determined by the number of particles, but also by the outer form of the system.

In order to investigate the melting process of the nano-structure given in Fig.1 and Fig.2 we increased the temperature (Fig.3). It turned out that a melting temperature is not or hardly defineable because the sublimation of the system is faster than the melting process, that is, the melting process is overtaken by the sublimation process and, therefore, melting does not take place.

In conclusion, specific material properties of nano-systems can be essentially different from the corresponding properties of macroscopic systems. This has been demonstrated in connection with the thermal stability and the melting temperature of the nano-structure shown in Fig.1.

An essential reason for this tendency is the fact that a great fraction of the particles (atoms, molecules) of such small systems belongs to the surface region, and the surface particles are less bonded than the particles in the bulk, leading to relatively strong anharmonicities already at temperatures far below the melting point. Even the melting process takes place far below the bulk melting temperature, or is simply not defined as has been demonstrated in connection with the nano-system shown in Fig.1, Fig.2 and Fig.3. The thermal behaviour of such systems is a complicated function of particle number and the outer shape of the systems. This must have consequences for the theoretical description of the material properties for systems of nanometer-size. We will discuss this point in more detail elsewhere.

III. FINAL REMARKS

Materials research at the nano-level requires not only making use of conventional solid state physics[3,4], which is based on an ordered structure and the harmonic approximation, but, due to the strong anharmonicities and the strongly disturbed structure of nano-systems already far below the melting temperature, statistical mechanics and the theory of liquids (see, for example, Refs.[5-7]) are also needed. In this connection molecular dynamics calculations are of considerable importance, and up to now there is obviously no alternative to this method.

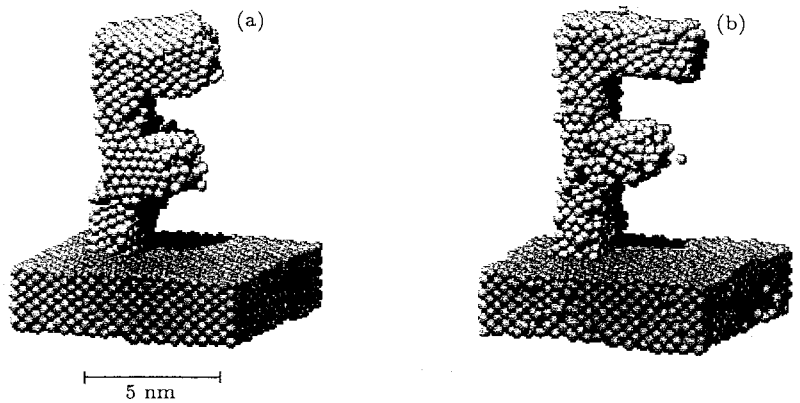


Fig.2. A slight variation of the initial conditions can lead to different final shapes of the nano-system. In (a) the temperature is 400 K after 10^4 time steps; in (b) the temperature is 500 K after 5000 time steps.

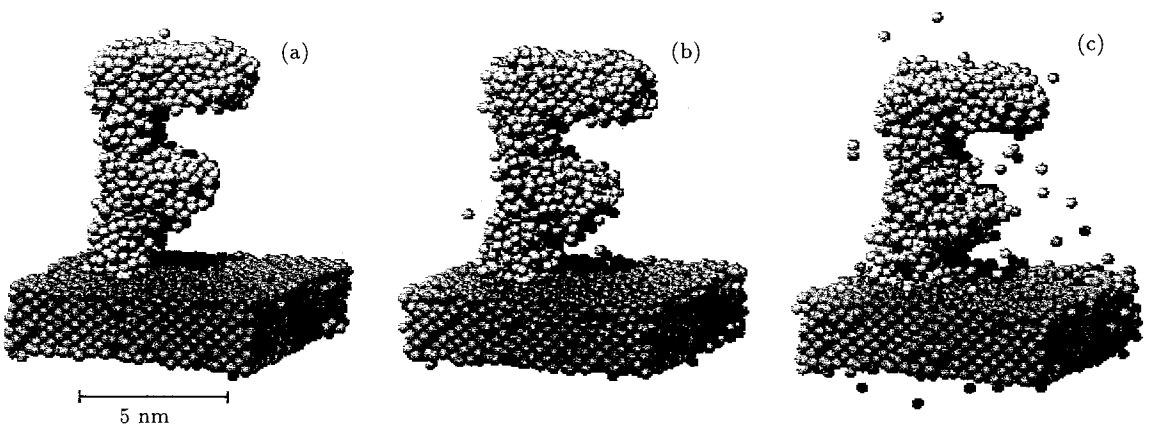


Fig.3. In order to investigate the melting process of the nano-structure given in Fig.1 and Fig.2 we increased the temperature using configuration shown in Fig.2(b). In (a) of the figure the temperature is 600 K, in (b) the temperature is 750 K after 1000 time steps, and in (c) the temperature after 4000 time steps is still 750 K. It turned out that a melting temperature is not defineable because the sublimation of the system is faster than the melting process, that is, the melting process is overtaken by the sublimation process and, therefore, melting does not take place.

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