THE COMPUTER MODELS OF 12 AND 13 ATOMS CLUSTERS FOR LITTLE METALLIC AGGLOMERATIONS

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As it was shown in a precedent computer model of 7 atoms clusters [1], we used a Monte-Carlo method, in order to simulate the first phases of thin film formation process. We remind that this experiment is performed in the following way: an initial cluster of atoms is build in a limited space region of 5Å, choosing randomly the coordinates of a new arrived atom, by means of a special random number generator. Then we calculate the potential energy related to the next neighbouring atoms using the Lennard-Johnes potentials which appeared to be very useful for the simulation experiments performed by Johnson [4] on α-Fe structural defects:

$$V = A\left(\frac{r_0^{\,6}}{r^6} - \frac{r_0^{\,12}}{r^{12}}\right) \tag{1}$$

These experiments are performed for the atom groups having the nickel parameter (r_0=2,45 Å) and they present great interest for Sb, S, Se, Te, Ge, Si and many others covalent bond compounds [5].

With the same number generator, the atom is moved next in a random x,y,z direction and by a random limited distance and the potential energy is again evaluated. The new atom position is retained only in the case of energy minimisation. Elsewhere, it takes place a new random move of the atom. All the atoms of the proposed structure suffer the same treatment. The final cluster structure is the result of the absolute energy minimisation.

To see the result of simulation we represented the radial distribution function (RDF), namely the number of atoms on y-axis versus the distance between all next neighbouring atoms on x-axis, at the beginning and at the end of computer experiment.

We simulated also a twelve atoms initial cluster. In this case the number of all possible configurations is considerably higher. The essential problem is to investigate if the pentagonal configuration presents even now a minimum of energy. If we use an initial random positioning for atoms we obtained a non-crystalline structure presenting a pentagonal symmetry. But, if we begin with an initial cluster with all twelve atoms arranged in a strict c.c.p.–crystal arrangement, and using an initial step of 0,15 Å, we are simulating the transition from crystalline phase to the non-crystalline one (see fig. 1). If we should calculate the number of all possible configurations presenting one atom in an

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erronate position, we found that the pentagonal structure should appear six times less than the trigonal one.

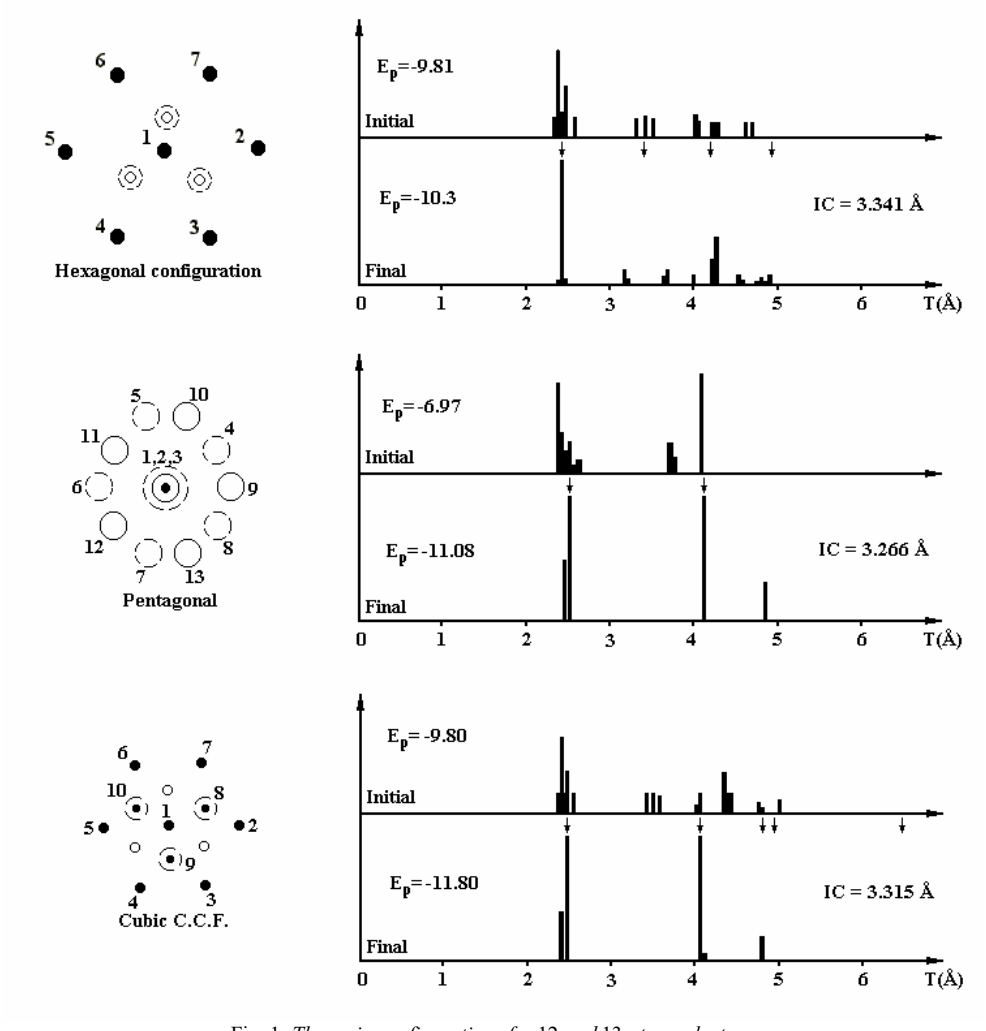

Fig. 1: *The main configurations for* 12 *and* 13 *atoms clusters.*

We concluded that such a little step of displacement was sufficient to simulate the migration energy necessary to the phase transition.

We tried also to begin simulation experiments with an initial 13 atoms cluster packed in a hexagonal configuration. As results from Fig. 1, the RDF shows that the energetic minimum is obtained also for a hexagonal configuration, but a little distorted. This proves that such an initial hexagonal configuration does not lead to the pentagonal packing. That would suggest that the hexagonal structure differs from the cubic one by a significant energy level. We expect also that in the thin films generation process the hexagonal clusters would appear first. They will be after preferentially transformed in a cubic c.c.p.–phase

rather than in the hexagonal one due of course to the higher energy level. We tried also to begin in the experiments with an initial atom cluster packed in a hexagonal configuration.

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Conclusions

In this computer simulation we deal with some more energy minimums. The lowest level of energy corresponds to pentagonal structure – the most stable configuration in this process, but incompatible with a translation operation.

The next structure of the energy level is that of cubo-octahedric crystalline configuration which can be extended, in the whole space.

This explains why the non-crystalline phase can be obtained from the vapour phase, only in very restricted conditions: the energy of the deposited atom must be quickly taken by a cold support and in this way the migration should take place only on small distances. In this way the formatted condensed germs could not be sufficiently great to favour one of the crystalline configurations. Conversely, a higher temperature support expects the crystalline structure formation. If the deposition conditions permit, the problem is which crystalline phase type should appear preferentially. In the first stage of the process, the cubic phase is proved to be more favourable than the hexagonal one. If the surface of the substrate is very clean, the interaction between it and the arriving atoms should be very strong and in this case the number of condensing centers presenting an octahedric pyramidal configuration is increased much more than the trigonal (tetrahedric) centers [9]. In this case, the cubic structure is favoured and the growing of crystallites is predominant in the (100) orientation.

In this way it was proved that the experimental conditions and the participation of different phase structures with different energy levels determine the thin film final structure.

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