VIBRATION INDUCED CRYSTALLIZATION OF AMORPHOUS MATERIALS: MOLECULAR DYNAMICS STUDY

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This is the first systematic research on the crystallization phenomena induced by external vibration using molecular dynamics simulation of Lennard-Jones molecules. External cyclic forces with a dc bias are superimposed on the intermolecular forces, which govern the global behavior of molecules. In the course of this study it is discovered that external force fields can induce crystallization effectively without heating problem, RDF is sufficient to observe the crystallization process and the crystallization propagation speed can be estimated when the amorphous material is exposed to the external force field locally.

Efficient fabrication technology of poly-Si thin-film transistors (TFT) at a low temperature has long been demanded and developed for use in photovoltaics, microelectronics, and display devices of larger area and high-quality, since a low temperature process overcomes problems involved in amorphous Si TFTs and ploy-Si TFTs fabricated at a high temperature. There are several processes practically available to fabricate poly-Si thin film at low temperatures including PECVD (plasma enhanced chemical vapor deposition), MIC (metal induced crystallization), ELC (Eximer laser crystallization), PRTA (pulsed rapid thermal annealing), etc.

Very recently it has been shown that an alternating magnetic induction process can bring about more effective crystallizations of a-Si on a glass substrate at temperatures below 500 °C, which promises the crystallization of larger areas and faster processing without metal contamination. The mechanisms for the alternating magnetic field crystallization (AMFC) are not clearly understood yet. It is conjectured that the AMFC is due to heating of a-Si by eddy current losses in an alternating magnetic field or due to oscillation of some portion of molecules by electric fields induced by the magnetic field. The first hypothesis is proven not to be relevant, since the film temperature remains almost constant during the crystallization process and a theoretical simulation indicates that the process temperature is too low to increase the temperature of a-Si up to effective annealing temperatures. The second hypothesis will be tested in this study to understand the crystallization mechanism and to optimize the control parameters for its process. There are not many theoretical tools available to examine the second hypothesis. Therefore, it is decided to apply the MD technique to the numerical experiment whether externally forced molecules will cause crystallization or not, although the forced molecules are selected randomly and the external forces are artificially imposed.

A crystalline structure and RDF obtained from the fcc structure of solid argon is equilibrated at $T^* = 0.496$ as shown in Fig. 1. Although the peaks for the crystal at $T^* = 0.496$ are much smaller than those of the reference fcc, the behaviors are quite similar to those of the reference. The temperature of the solid equilibrated at $T^* = 0.496$ is suddenly raised up to $T^* = 2.48$ and the volume has been slightly expanded to easily obtain the amorphous structure and to prevent the molecules from being gasified. This amorphous structure is again cooled down to $T^* = 0.496$ to obtain an amorphous structure. The supercooled liquid from the supercritical fluid is equilibrated at $T^* = 0.496$ over 100000 steps and the molecular distribution and its RDF are shown in Fig. 2.

Figure 3 shows the variation of the RDF's from time step 0 to 62000 during vibration-induced crystallization process and recrystallized molecular structure. The abrupt increases of the second and third peaks are clearly and simultaneously detected near 40000 steps, which imply that the material is undergoing the crystallization process, although the creation or destruction of crystalline nuclei cannot be detected.

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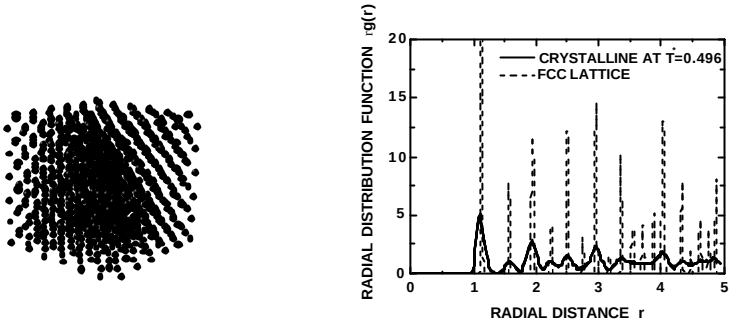

Fig. 1. Molecular distribution and RDF for crystalline structure at $T^* = 0.496$.

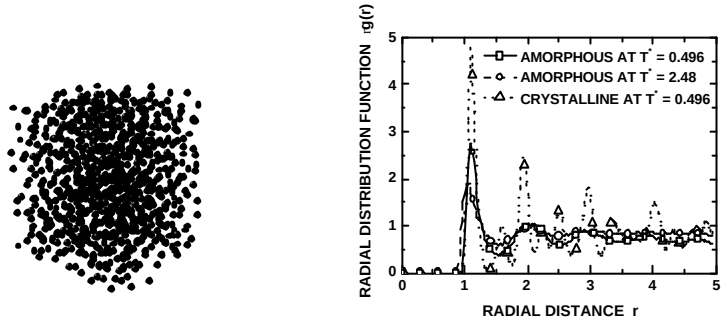

Fig. 2. Molecular distribution and RDF for amorphous structure at $T^* = 0.496$ and 2.48.

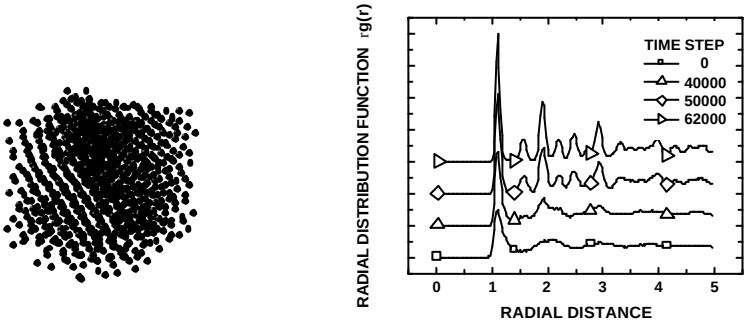

Fig. 3. Recrystallization induced by external vibration: molecular structure and the variation of RDFs with respect to time at $T^* = 0.496$.