Radiation-induced glass transition and structural fluctuation in NiTi metallic glass system

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Spatio-temporal nanostructural fluctuations brought about by transient, metastable atom-cluster formation and the manifold nature of inherent atomic ordering in electron-irradiation-amorphized NiTi were investigated by using a combination of *in situ* observations inside a high-resolution high-voltage electron microscope (HR-HVEM) and image analyses of molecular-dynamics-simulated atom configurations. Nanometer-sized clusters were found to appear and disappear in the irradiated region. The random formation and annihilation of such nanoclusters are believed to be responsible for nanostructural fluctuations which appear to be related to transitions among manifold inherent structural states, involving multi-relaxation processes.

Figs 1(a) and (b) show the experimental and simulated HR-HVEM images, respectively, at various dose levels during irradiation at room temperature [1,2]. The specimen orientation was <111>, as is the electron incidence direction. During the amorphization process, nanosized atom clusters were seen to repeatedly form and annihilate in the images (some of them are indicated by the circles). Correspondingly, extra spots appeared and disappeared in the diffraction patterns. The response of the compound to irradiation in the MD simulation can be summarized as follows: chemical disordering occurs progressively after a short irradiation time, and then topological disordering begins and proceeds until amorphization is completed.

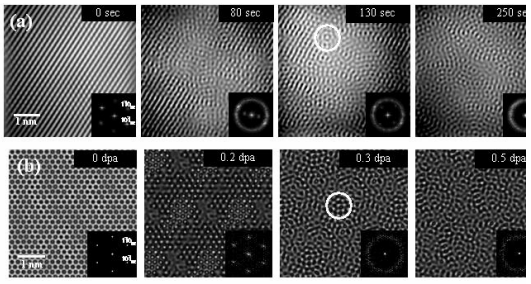

Fig. 1(a) High-resolution images and FFT patterns obtained by HVEM experiment at 300K. (b) Calculated atomic structural images and diffraction patterns by MD simulation.

The fact that chemical disordering precedes topological disordering and that chemical disordering alone cannot trigger amorphization in this alloy implies that the sequence of the two disordering processes is necessary for inducing amorphization as well as for the observed diffuse scattering. In fact, between the chemical and topological disorder states, the total potential energy of the system increases continuously with concurrent fluctuations, and saturates upon complete amorphization. This implies that sequential disordering is intrinsically a deterministic process in amorphization, although structural fluctuations due to metastable atomic-cluster formation can be stochastic events.

Temporal fluctuations during irradiation were manifested through the dose-dependent local amorphization parameter in the calculated potential energy and volume change. The random formation and annihilation of such inherent nanoclusters are believed to be responsible for these fluctuations.

The observed fluctuations (α =0.1~0.3) seem to obey a universal power law: $S(f) = A \cdot f^{-2+a}$ for power spectra and $y(t)/y(0) = 1-(t/t_0)^{1-a}$ when $0<\alpha<1$ for the autocorrelation function [3]. The power-law behavior found in the structural fluctuations suggests that the irradiation field in an HVEM can provide a means to explore nonequilibrium open systems. The present results also suggest that our irradiated compound be a self-organized-criticality system. The present author has also been investigating such power-law fluctuations in this amorphous material from the view point of multi-Lorentzian spectral model [4].

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