Characterization of pressure-induced amorphous silicon

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Keywords: amorphous silicon, nanoindentation, fluctuation electron microscopy, medium range order.

The behaviour of crystalline silicon (c-Si) under high pressure has attracted interest for decades now and has been studied extensively by both diamond-anvil cell [1] and indentation experiments [2]. It is well known that c-Si undergoes a phase transformation to a metallic silicon phase, Si-II, on loading. In indentation experiments, this phase transforms upon pressure release to either the crystalline high-pressure phases Si-III and Si-XII or to an amorphous phase, the so-called pressure induced (PI) amorphous silicon (a-Si). This differs significantly from diamond-anvil cell experiments where the formation of a-Si has not been observed at room temperature. However, little is known about the structural properties of this form of a-Si and thus, this study addresses these issues.

Nanoindentation itself (by re-indentation within a previously indented region) is one way to determine the mechanical properties of these various phases of silicon. A relatively large volume (9 μm diameter extending approximately 400 nm below the surface) of the PI a-Si can be created in a crystalline substrate by indentation using a microscale tip. This material can then be probed in turn by indentation using a nanometer scaled Berkovich tip allowing sampling of the top 150 nm. Such mechanical testing does not only give information about properties such as hardness or elastic modulus, but in the case of silicon also about the possible phase transformation behaviour.

Characteristic indentation load-displacement curves from as-prepared and relaxed (annealed at 450ºC) PI a-Si will be reported. These indentation results are correlated with Raman microspectroscopy, cross-sectional transmission electron microscopy (XTEM) and fluctuation electron microscopy (FEM).

We found that annealing changes the deformation behavior of PI a-Si significantly in that the as-indented PI a-Si deforms via plastic flow, whereas relaxed PI a-Si phase transforms in a similar way to c-Si, as shown in the XTEM images in Fig. 1. This behavior is compared to the indentation behavior of relaxed and unrelaxed ion-implanted a-Si that we have reported previously [3]. While diffraction experiments have not been able to discern striking differences between the structures of as-prepared and relaxed a-Si, FEM demonstrates, as shown in Fig. 2, that the relaxed a-Si structure approaches a perfect continuous random network, while the as-prepared a-Si exhibits a much higher degree of medium range order (MRO) in the case of ion-implanted a-Si and a much lower degree in the case of PI a-Si [4]. These intriguing differences in MRO might be attributable to differences in mass-density between the as-prepared amorphous networks.

W. Grogger, F. Hofer, P. Pölt (Eds.): MC2009, Vol. 3: Materials Science,
DOI: 10.3217/978-3-85125-062-6-639 , © Verlag der TU Graz 2009

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5. This work was supported in part by the US Department of Energy under contract number DEAC02-06CH11357 at Argonne National Laboratory. The FEM and EELS was conducted in the Electron Microscopy Center at Argonne National Laboratory. Funding provided by the Australian Research Council is also gratefully acknowledged.

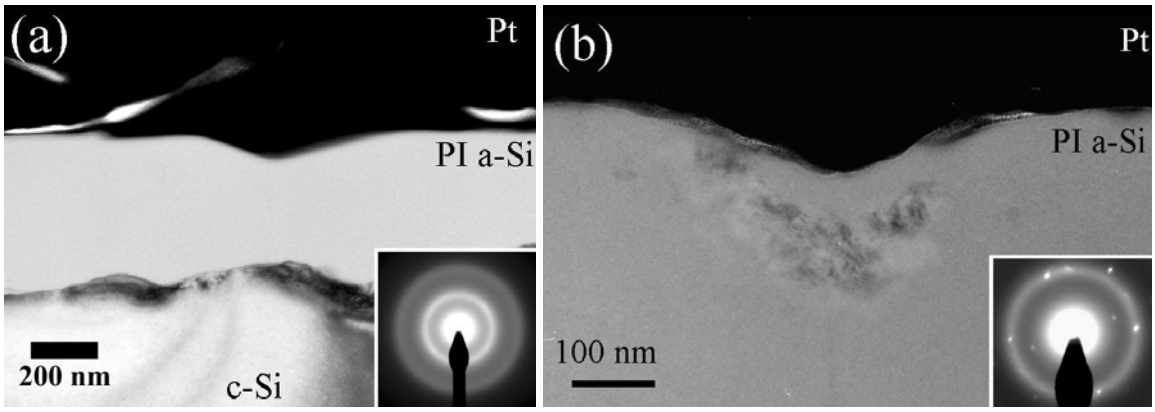

Figure 1. Bright-field images of TEM cross-sections made through residual indents in (a) as-induced PI a-Si and (b) relaxed PI a-Si. An SADP taken from beneath the residual indent is shown as an inset in each case.

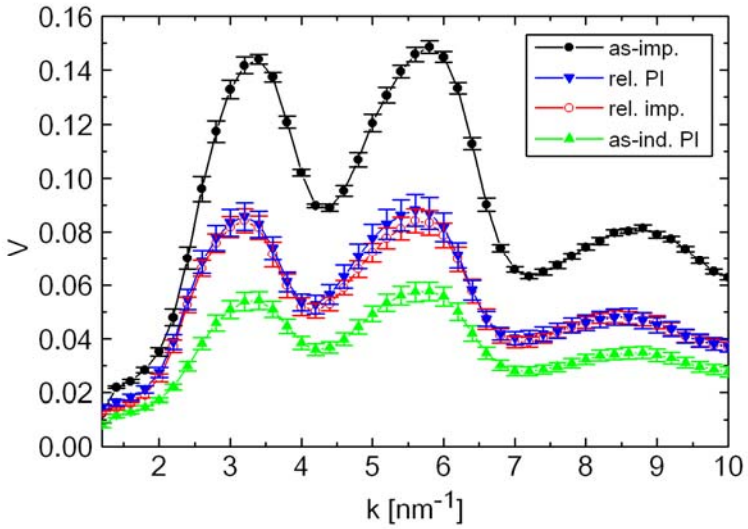

Figure 2. Variance as a function of k, i.e. the MRO of the different forms of a-Si.