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Combined EXAFS and MD study to elucidate defect behaviors and stage IV recovery mechanism in heavy ion irradiated molybdenum

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ABSTRACT

The microstructural behaviors of materials control material properties and the recovery mechanism is a key to understanding the microstructural changes induced by irradiation. But the recovery mechanism of many metal materials is not fully understood through traditional research methods. By using Extended X-ray absorption fine-structure (EXAFS) measurements combined with Molecular Dynamics (MD) simulations, we studied the stage IV recovery process through investigating the behaviors of irradiation induced defects (caused by 104 MeV xenon ion beam irradiation) at an elevated temperature (~350 °C) in single crystal Molybdenum (Mo). We distinctly characterized self-interstitial dumbbell defect configurations and simulated their behaviors at this elevated temperature. EXAFS measurements, together with MD simulations and TEM observations, revealed that the mechanism of IV stage recovery is the migration of interstitial type defects (including dumbbells) rather than vacancy type defects. We also discussed the possible states of dumbbells after the stage IV recovery. These results further revealed the nature of the irradiated BCC structure (Mo).

1. Introduction

Evolution of defects induced by irradiation and their collective behaviors have marked effects on the properties of metals [1-2]. Understanding such behaviors from the atomic level is extremely necessary to the understanding of material degradation mechanism under irradiation [3]. Researchers have conducted in-depth studies on irradiation effects of a variety of metals [4-7] for decades. Recovery, described as defects annihilating with each other at a certain temperature regime, is a very important process in which ample amount of defect evolution information are embedded. Recovery process can be divided into several stages according to the melting point and recovery temperature of the metals [8-11]. The underlying physical recovery mechanism at each stage is like a treasure that researchers have been tirelessly hunting for [3,12-15]. Because molybdenum (Mo) with body-centered-cubic (bcc) structure is expected to be widely used in practical engineering applications (for example, it is regarded as a candidate material for accident tolerant fuels [16-17]) due to its excellent physical properties (high melting point, good thermal conductivity, good resistance to corrosion, etc. [18-22]), it is usually selected by researchers as a key research object. In electron irradiated Mo, there are only three recovery stages [9,23-25]: temperature below 120 K is associated with stage I; temperature of 120K-350 K is associated with stage II and temperature of 330K-600 K is stage III.

It appears that all the defects induced by electron bombardment can recover completely at stage III. When the defects are induced by neutron or heavy ion irradiation, however, stage III is followed by a stage IV at about 600K-900 K [26] and even a stage V recovery [27]. The recovery mechanisms of the first three stages (i.e. stage I, II and III) of Mo upon electron irradiation had been clarified by researchers [9,23-24,28-35]. Summarizing the recovery mechanism of the electron irradiation, Frenkel pairs are created and then annihilate with each other in stage I recovery. Interstitial atoms migrate until they are trapped by impurities or annihilate at vacancies once the temperature is above 50 K [24].

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