Conf-811150--15

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DE83 007794

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Wayne E. King and R. Benedek

Materials Science Division
Argonne National Laboratory, Argonne, IL 60439

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*Work supported by the U.S. Department of Energy.

Manuscript submitted to the Yamada Conference V on Point Defects and Defect Interactions, Kyoto, Japan, November 16-20, 1981.

MOLECULAR-DYNAMICS SIMULATION OF DISPLACEMENT CASCADES IN Cu: ANALYSIS OF REPLACEMENT SEQUENCES

Wayne E. King and R. Benedek

Materials Science Division, Argonne National Laboratory Argonne, Il 60439, USA

Molecular-dynamics computer simulations of displacement cascades in copper have been performed for recoil energies up to 450 eV. Statistical analyses of the atomic replacements are presented. Linear replacement sequence lengths are extremely short on the average. The effect of the cooling phase of the cascade is discussed.

The role of atomic replacement sequences in energetic displacement cascades has long been a matter of controversy. A number of experiments have been interpreted in terms of long range focussed replacement sequences but the efficiency with which these sequences are produced has not been reliably established [1]. Several approximate analytical treatments of replacement sequences are given in the literature [2,3]. Computer simulation techniques including molecular dynamics, [4,5,6,7] "quasi-dynamic" methods [8], and binary collision approximation [9] have also been applied. In principle the molecular dynamics approach [4] is the most rigorous, but it has been used somewhat sparingly in the past. One advantage of molecular dynamics is its capability of treating not only the displacement spike, or collisional phase ($\sim 10^{-13}$s) of a cascade (to which the other techniques are restricted) but also the much longer thermal spike or cooling phase ($\sim 5 \times 10^{-12}$s) during which many atomic rearrangements can occur.

In the present work, molecular dynamics simulations have been applied to study displacement events in copper for an extensive set of primary knock-on atom (PKA) directions and energies (up to 450eV). Results of analyses of the replacements in these events are presented here; the analysis of Frenkel-pair production is described in another article in these Proceedings [10]. One of the principal results of this study is that on the average, linear replacement sequences are very short (<2 replacements for PKA energies > 100eV). Furthermore, a substantial fraction of all atomic replacements lie in closed chains (referred to as "ring interchange" by Gibson et al. [4]) Thus, whereas the total number of replacements per event observed in the simulations is of the same order of magnitude as that derived from thermal neutron experiments on Ni_3Mn [11], the spatial arrangement of the replacements is quite different from what is normally assumed (i.e. a small number of long linear replacement sequences). Many of the replacements occur during the cooling phase of the cascade and, consequently, the final arrangement of the interstitials and vacancies often bears little resemblance to the arrangement at the end of the displacement spike.

Simulations were performed using a modified version of the SUPERGLOB code [12] for 14 PKA energies in the range $25 \leq T \leq 450$eV. The Gibson II potential was used to represent the atomic interactions [9]. For PKA energies <150 eV, a cubic computational cell of size 10a on each edge was employed, with a lattice constant a=3.608Å for copper. At higher PKA energies, cells of dimension 12a were used.

Several events at 250 and 300 eV were also run in a cell of dimension 16a. Thermal vibrations were not included. The end of the collisional phase of an event is defined here as that time at which all atomic energies in the cell have fallen below 5eV. Replacements are analyzed at the end of the collisional phase and at the end of the event ($\sim 5 \times 10^{-12}$s). A replacement is considered to occur on each lattice site (Wigner-Seitz cell) that is occupied by an atom other than the one originally located on that site; multiply occupied sites (interstitials) are not included. Two types of replacement "chains" were observed: "open" chains, bounded on one end by a vacancy and on the other by an interstitial, and "closed" chains in which replacements form a closed loop (ring interchange). Most chains consist of several distinct linear replacement sequences, connected end to end. Events in which an atom propagated into the cell boundary were not included in the statistical analyses presented below. For the set of PKA directions shown in Fig. 1, one such event occurred at T=400 eV and four occurred at T=450 eV.

The results given below represent averages for the 18 directions indicated in Fig. 1. Figure 2 shows the mean number of replacements per linear sequence in the three principal symmetry directions. Linear sequence lengths are quite short. The decrease in mean <110> sequence length for T>50eV is due to defocusing effects [9]. The results for <222> sequences reflect the rather large replacement and focusing energies in this direction. By far the greatest number of replacements at all energies are of the <110> type as shown in Fig. 3. The short mean sequence lengths (Fig. 2) are a result both of the large number of replacement "sequences" of minimum length, i.e. isolated replacements (Fig.4) and of the short maximum linear sequence length per event (Fig.5).

Figure 6 shows the mean total number of replacements per event as a function of recoil energy. At energies $\gtrsim$100eV, the number of replacements at the end of the event is about twice that at the end of the collisional phase. This result attests to the importance of the cooling phase of the cascade in determining the final arrangement of the defects and replacements. The cooling phase rearrangements are even more extensive than appears in Fig. 6, since many collisional phase replacements are "undone" later in the event, e.g. by recombination.

In Fig. 7 we observe that for T $\gtrsim$ 75 eV about 60% of the chains are closed. These rings of replacements are remnants of transient Frenkel pairs that recombined during the cooling phase of the cascade; no closed chains exist at the end of the collisional phase. The mean length of closed chains is relatively constant for T$\gtrsim$125 eV , however, the length of open chains increases with energy (Fig. 8).

Figure 9 shows defect distributions for a 250eV event, which illustrate some characteristic features of cascades. Vacancies are represented by spheres, interstitials by ellipsoids, and replacements by points. At the end of the collisional phase (Fig. 9a), $\sim 2.0 \times 10^{-13}$s, 15 replacements were observed in 7 open chains. The longest linear sequence was 5 replacements in the <100> direction. At the end of the cooling phase (Fig.9b) a total of 34 replacements was observed. The longest linear sequence was 4 replacements. The two open chains have an average of 11 replacements each, whereas the 3 closed chains have an average of 4 replacements each. This event illustrates the large amount of atomic mixing that occurs during the cooling phase of the cascade.

The present simulations indicate that average linear replacement sequence lengths in Cu are extremely short. This does not mean of course, that long linear sequences cannot occur (e.g. for a PKA with appropriate energy and orientation) but rather that long linear sequences are statistically rare in cascades. Since we have deliberately excluded directions close to the principal axes from our set of PKA directions (Fig. 1), our results pertain mainly to "secondary" or "cascade" sequences [9] i.e. sequences not directly initiated by the PKA. Such secondary sequences dominate the statistics, except at low PKA energies.

The simulations also demonstrate that rearrangements and atomic transport in the cooling phase of the cascade are quite extensive. The total number of replacements at the end of an event is on the average approximately twice as large as at the end of the collisional phase.

Work supported by the U. S. Department of Energy

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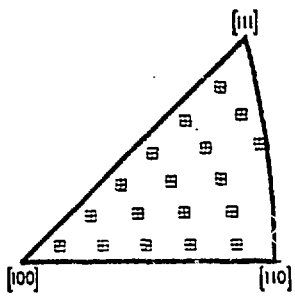


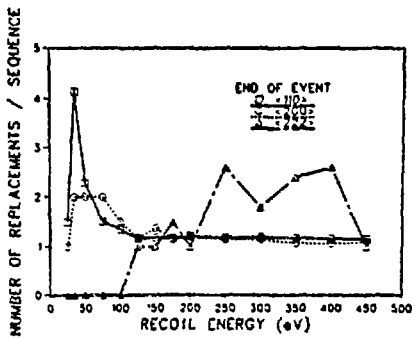
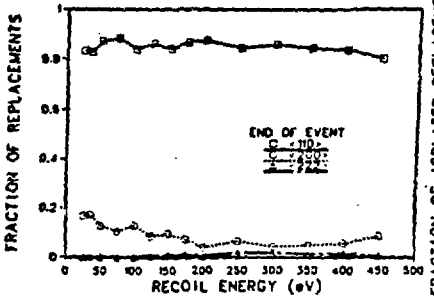


Fig. 1 18 PKA directions employed in present simulations.
Fig. 2 Average linear replacement sequence lengths in the three principal symmetry directions.



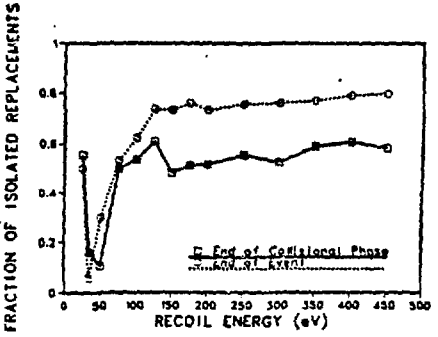
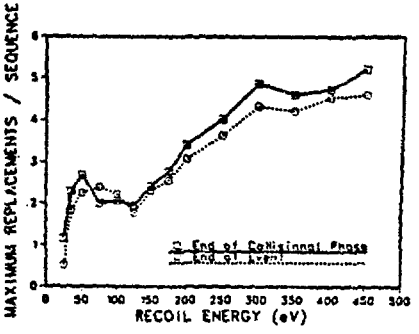


Fig. 3 Fraction of replacements of the <110>, <200>, and <222> types.

Fig. 4 Fraction of isolated replacements at the end of collisional phase and at end of the event.



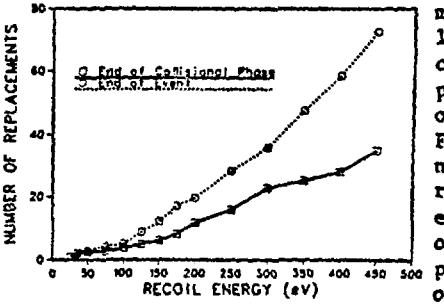
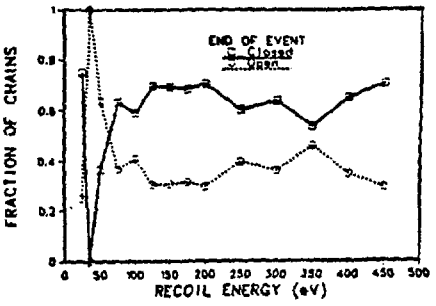


Fig. 5 Average maximum sequence length at end of collisional phase and at end of event.

Fig. 6 Mean number or replacements per event at the end of collisional phase and at end of the event.



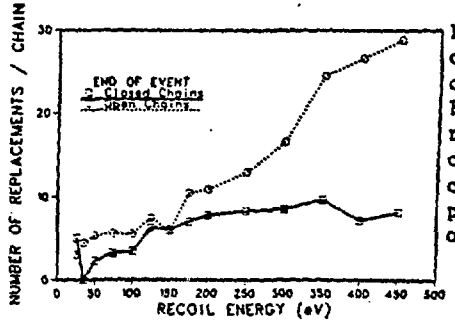
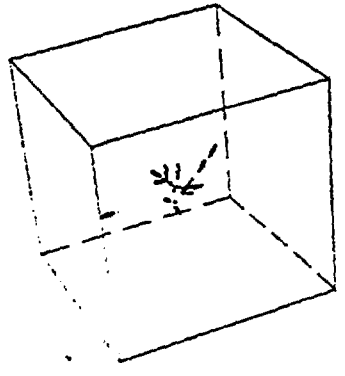


Fig. 7 Fractions of open and closed chains.

Fig. 8 Number of replacements per chain at end of collisional phase and at end of the event.



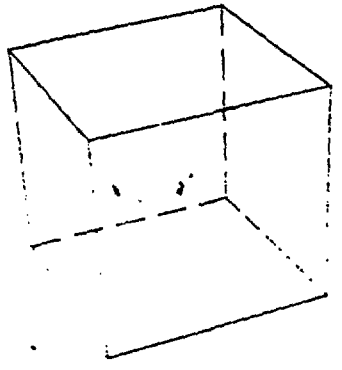


Fig. 9 Defect distributions for a 250eV event (a) At end of collisional phase and (b) At end of event. Box represents size of computational cell