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Structure of nanoscale copper precipitates in neutron-irradiated Fe-Cu-C alloys

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The structure of copper nanoclusters/precipitates formed under neutron irradiation in Fe-0.3 wt. % Cu-C alloy is studied by the internal friction and positron annihilation experiments of postirradiation annealed alloys. The appearance of a carbon-relaxation peak during the first recovery stage at about 723 K reveals the fact that complex carbon-vacancy-copper clusters have formed during the irradiation-mediated copper precipitation process. The stability of Cu-C-vacancy clusters is confirmed by *ab initio* calculations. The existence of a structural phase transition of copper precipitates is observed in the alloys that are annealed at temperatures between the first and second recovery stages, which indicates that the dissociation of vacancies and carbon atoms from the vacancy-copper-carbon clusters is accompanied by the crystallization of Cu precipitates.

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I. INTRODUCTION

The structural properties of nanoclusters formed under neutron irradiation in iron-based alloys hold key information relevant for understanding embrittlement of reactor pressure vessel (RPV) steels. Among the variety of solute, vacancy, and interstitial clusters, and their mutual complexes, the nanoscale copper precipitates are so far recognized as main ingredients of irradiated steels that exhibit an enhanced increase of strength and embrittlement.[1–3] This originates from the fact that initially absent copper precipitates appear under irradiation and represent obstacles to the dislocation motion.[4–7] Due to the low solubility of Cu in Fe, copper precipitates are formed relatively easily in Fe-Cu binary alloys subjected to elevated temperatures, application of stress, irradiation, and so on. In contrast to the precipitates formed by thermal aging, which are experimentally extensively studied,[8–13] irradiation-induced Cu precipitates in materials with copper concentrations relevant for applications in structural nuclear materials (up to 0.3 wt. %), are extremely difficult to resolve by transmission electron microscopy due to their small sizes. In particular, no information about their crystallographic structure is available, although they are assumed to have the same structure as the matrix, i.e., bcc. The main difference between the Cu precipitates formed by neutron irradiation and by thermal aging in FeCu binary alloys is established on the basis of positron annihilation spectroscopy (PAS) studies. It has been shown that in the former case the Cu-vacancy complexes aggregate into Cu-coated voids,[14,15] while in the latter it is argued that the Cu precipitates consist of only Cu atoms and are free from open-volume defects.[13] There are two issues related to these observations that we would like to address in this work.

Experiments and *ab initio* calculations have shown that a strong affinity between the carbon atoms and vacancies exists.[16–18] Since carbon is always present in Fe alloys, the PAS findings suggesting the formation of Cu-vacancy clusters raise the question of whether such complexes will also include the carbon atoms, even though Cu in itself is not an element that exhibits any special affinity to carbon (it is not a carbide former). An interesting recent result showed that carbon redistribution occurs in concomitance with the copper precipitation process mediated by neutron irradiation.[19] In neutron-irradiated Fe-Cu binary alloys, the existence of carbon redistribution is observed through the change of the carbon-dislocation relaxation process (Snoek-Köster-relaxation[20,21]) as a function of irradiation dose. However, the carbon destination(s) and/or redistribution pathways are not understood.

The presence of large vacancy concentration in copper precipitates questions the existence of crystalline lattice of the precipitates. This is in contrast with the Cu precipitates formed under thermal aging. In thermally treated supersaturated Fe-Cu solid solution, it is well established that the crystalline structure of Cu precipitates evolves through different phases (bcc-9R-fcc) depending on the precipitate size, as a result of bulk instability prevailing the influence of the cluster interface.[8] Unfortunately, no technique provides the possibility of studying crystallinity of Cu precipitates created under neutron irradiation, leaving an open question in that respect for neutron-irradiated Fe-Cu alloys. Most recently, low-temperature internal friction spectra and specific heat measurements of thermally aged Fe-1 wt. % Cu alloys[22] showed that Cu precipitates exhibit a structural phase transition at $T_c = 122$ K. Even though the precise precipitate structure below T_c is not yet determined, the bare existence of this phase transition provides an excellent probe of the precipitate crystallinity.

In this study, we perform IF and PAS measurements of postirradiation isochronally annealed Fe-0.3 wt. % Cu-C alloys to investigate the possibility for carbon to associate with Cu-vacancy clusters in irradiated Fe-Cu alloys. We also attempt to determine the degree of crystallinity of Cu-vacancy clusters. The two observed recovery stages, one at about 723 K, corresponding to the vacancy dissolution, and at 923 K corresponding to Cu precipitate dissolution, are in good agreement with previous results.[14] The appearance of the carbon relaxation peak in the temperature-dependent IF spectra correlates with the first recovery stage. This suggests the formation of carbon-vacancy-copper clusters during irradiation. These clusters deliver carbon back to the iron lattice on annealing. Most interestingly, the existence of structural phase transition at 122 K is observed only in neutron-irradiated alloys that are thermally annealed in the temperature range between the first and second recovery stages. Since the vacancy and carbon atoms have been removed from the precipitates during the first recovery stage, the Cu precipitate crystalline structure forms, resembling that of the precipitates in thermally aged Fe-Cu. In order to justify the conclusions obtained through experimental data, in particular to elucidate whether Cu-vacancy-C interaction indeed can take place, we performed a set of *ab initio* calculations.

II. EXPERIMENT

The material used in this study is polycrystalline Fe-0.3 wt. % Cu-C alloy with about 30–50 ppm C. The neutron irradiation was performed in the Belgian Reactor (BR2) up to a dose of 0.1 displacement per atom, dpa (6.9×10^{19} n/cm^2), at the temperature and pressure of about 573 K (300 °C) and 150 bar, respectively. The details of the sample preparation and irradiation conditions are published elsewhere.[15,19] The postirradiation isochronal annealing (0.5 h) was performed at various temperatures in the range between 573 and 973 K.

The internal friction measurements were performed in an inverted torsion pendulum[23] operating in free vibration at about 2 Hz (with a typical sample size of $1.3 \times 1.3 \times 30$ mm^3) in the temperature range between 100 and 600 K. From the free decay signal, the resonance frequency (modulus), ω, and the internal friction coefficient (damping), Q^{-1}, are determined. Q^{-1} is proportional to the ratio of the energy dissipated during one cycle to the maximum elastic energy stored in the sample. The measurements have been performed at a strain amplitude of about 10^{-4}, in a He atmosphere with a heating rate of about 1.5 K/min, and no magnetic field is applied.

The PAS experiments are performed with the coincidence Doppler broadening (CDB) and positron annihilation lifetime spectrometers (PALS). The CDB spectra are measured using two Ge detectors. Details of the setup are described elsewhere.[24] The CDB spectrum provides the momentum distribution of core electrons, which can be used to determine the chemical environment of positron-electron annihilation site.[25] The results are typically shown as the CDB ratio spectra, which correspond to the momentum distributions normalized to that of nonirradiated (defect-free) pure iron. The PALS measurements, which provide the size and density of vacancy type defects, are performed with a spectrometer[26] working in a triple coincidence mode with a time resolution of about 175 ps. The triple coincidence mode is used for irradiated materials in order to reduce the background originating from γ rays of the radioactive samples.

III. COMPUTATIONAL METHODS

A set of *ab initio* calculations is performed in the framework of the density functional theory (DFT) using the Vienna *Ab initio* Simulation Package (VASP).[27] The calculations employed Blöchl's projector augmented-wave (PAW) method[28] within the generalized gradient approximation (GGA)[29] and by applying the Vosko-Wilk-Nusair (VWN) interpolation.[30] The pseudopotentials were taken from the standard VASP library. The supercell approach with 3D periodic boundary conditions is used to calculate the optimum structure and corresponding formation energy of small C-Cu-vacancy clusters. Relaxation was performed in a supercell containing 250 atoms at constant volume using a lattice parameter of $a_0 = 0.2831$ nm. Brillouin zone sampling was performed using the Monkhorst and Pack scheme with 27 k points.[31] The plane wave cut-off energy was 300 eV. Such a parametrization set has been widely used in the past to compute properties of point defects and their small clusters in α-Fe (see, e.g., Refs. 17 and 32).

The binding energy (E_b) between two species has been calculated using a standard definition as a difference in the energy of a system containing two defects apart and together. Thus, a positive value of binding energy points that two species exhibit attractive interaction.

IV. RESULTS AND DISCUSSION

Figure 1 shows the IF spectra of postirradiation annealed Fe-0.3 wt. % Cu-C samples. Annealing temperatures are mentioned in the figure. All spectra are analyzed on the basis of standard Debye's relaxation expression:[33]

$$Q^{-1} \sim \Delta \frac{\omega\tau}{1 + (\omega\tau)^2}, \tag{1}$$

where ω denotes the angular frequency, Δ is the relaxation strength, and τ is the relaxation time $\tau = \tau_0 \exp(\frac{H}{k_B T})$ with the activation enthalpy H.

The IF spectra of Fe-0.3 wt. % Cu-C alloy annealed at 673 K and above this temperature exhibit a single peak centered at about 310 K. This peak is known as a

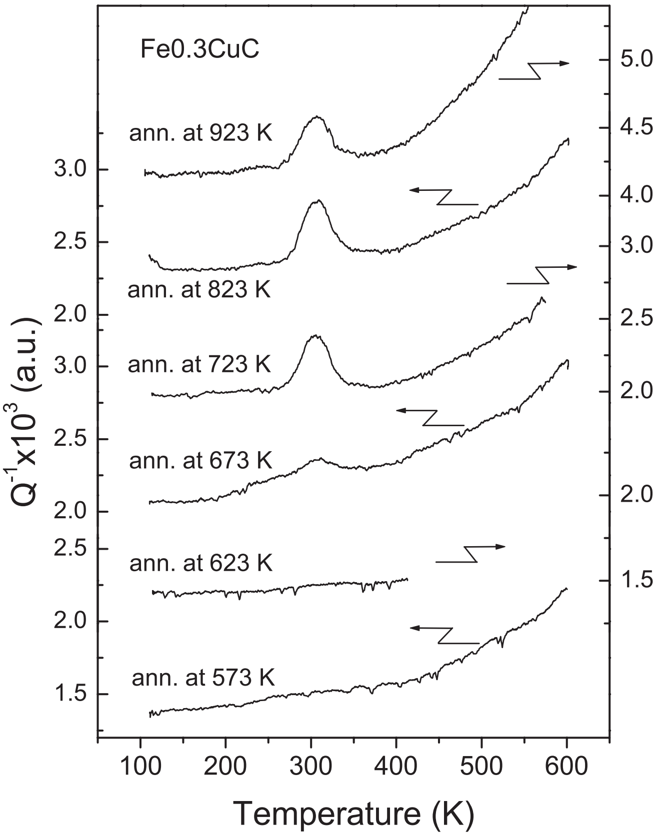

FIG. 1. Internal friction spectra as a function of the temperature of postirradiation annealed Fe-0.3 wt. % Cu-C alloy.

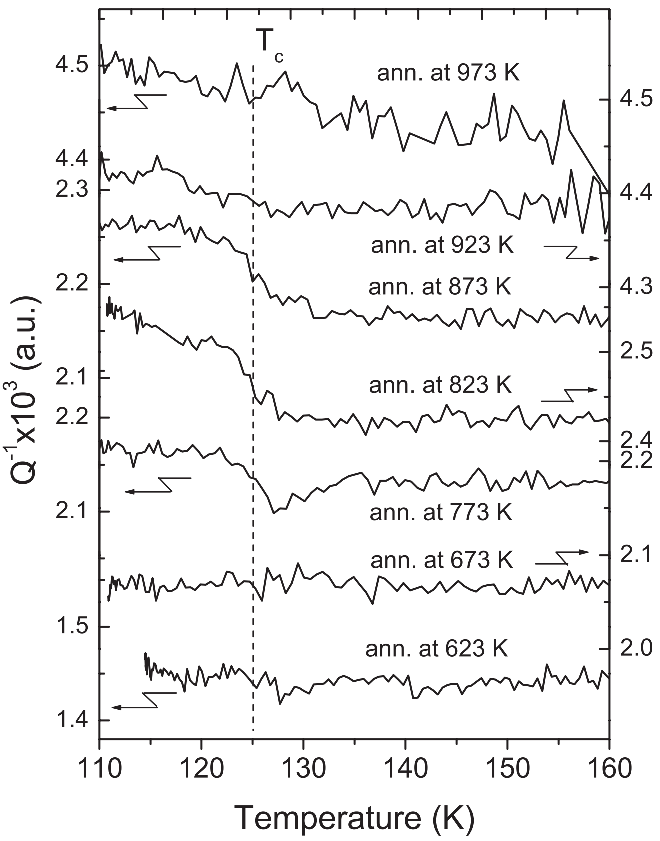

FIG. 2. Internal friction spectra in the temperature from 110 to 160 K of postirradiation annealed Fe-0.3 wt. % Cu-C alloy.

Snoek-relaxation peak and originates from thermal activation of carbon interstitals in the iron lattice. The overall peak shape, the temperature position, the activation enthalpy (0.89 eV), and the full width at half maximum (FWHM, ∼30 K) agree well with previous measurements[34] and are characteristics of point defect relaxation. The increase of annealing temperature causes rapid intensity increase of the Snoek peak, which reaches a saturation at about 773 K. The other two parameters, the peak position and FWHM, do not change as a function of the annealing temperatures. This behavior indicates that the carbon atoms are bound to neutron irradiation-induced defects that dissolve at the annealing temperatures above 673 K.

In addition to the Snoek peak, the IF spectra of alloys thermally annealed at 823 and 923 K show the existence of discontinuity, i.e., the steplike change of internal friction background at about 122 K; see Figs. 1 and 2. Such behavior of Q^{-1} typically indicates the existence of a phase transition. A similar anomaly at 122 K has been already observed in thermally aged Fe-1 wt.% Cu alloys and it is assigned to the structural phase transition of nanosize-Cu precipitates.[22] The origin of the phase transition is not yet fully understood, but since the bulk Cu (fcc) does not exhibit the structural change at 122 K, it is reasonable to assume that non-fcc Cu precipitates structurally transforms at 122 K. We believe that this phase transition is either related to the low-temperature transition of intermediate structure of Cu precipitates (such as 9R or 3R) or to the structural transition of the interface. A detailed view of this anomaly for different annealing temperatures is given in Fig. 2, where IF spectra are plotted in the temperature range from 110 to 160 K. Clearly, the discontinuity is only observed in alloys that are annealed in certain temperature range from 773 to 923 K. Moreover, in contrast to the IF spectra of thermally aged Fe- wt.% Cu alloys, where the phase transition is observed to be quite narrow (∼3–4 K), the phase transition in postirradiation annealed Fe-0.3 wt. % Cu-C alloys is much broader, i.e., the steplike change of the background spreads over 10 K. The broadening of the phase transition could originate from the precipitate size affecting the T_c, since at such small sizes the interface plays a great role in the energy of precipitate.

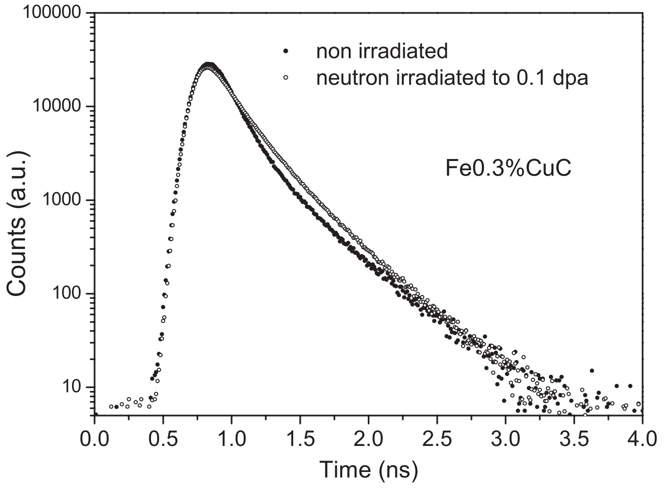

FIG. 3. Positron lifetime spectra of nonirradiated and neutron irradiated Fe-0.3 wt.% Cu-C alloy.

The PALS spectra of nonirradiated and neutron irradiated Fe-0.3 wt. % Cu-C alloys are shown in Fig. 3. The spectrum of irradiated material is normalized in such a way to give the same total number of counts (∼10^6) as for the nonirradiated material and analyzed by assuming the existence of two positron lifetime components. The effect of neutron irradiation is clearly seen by the appearance of a long positron lifetime component of about 230 ps, with the intensity of about 70%.[35] The short component is estimated to be of about 100 ps, which is close to the value in bulk Fe. These results differ somewhat from previously published results of Fe-0.3 wt. % Cu, where the values of two PALS components were found to be ∼300 ps and ∼160 ps.[14] Our value of 230 ps indicates that vacancy clusters contain about 5 vacancies in average, which is twice less than the size of clusters estimated in the previous study. Furthermore, our analysis shows the presence of less number of monovacancies that contribute to the positron lifetime of about 160 ps. However, the differences between results are not surprising, since neutron irradiations have been performed with different flux and fluence in these two experiments, as well as at different temperatures.

The CDB ratio spectra of postirradiation thermally annealed Fe-0.3 wt. % Cu-C alloys are presented in Fig. 4. The broad peak centered at about 25 × 10^{-3} m$_0$c, see Fig. 4(a), can be attributed to annihilation of positrons and 3d electrons of Cu atoms, in very good agreement with previous observations.[14] The enhancement in the low-momentum region is assigned to electron-positron annihilations at vacancies, voids, and

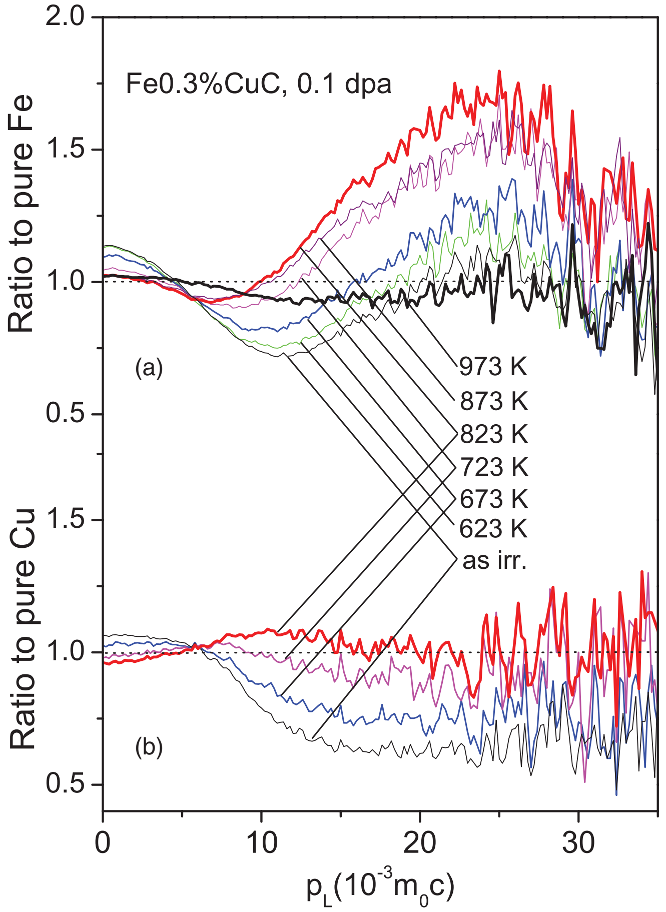

FIG. 4. (Color online) CDB ratio spectra with respect to (a) pure Fe and (b) pure Cu of post-irradiation annealed Fe-0.3 wt. % Cu-C alloy.

dislocation loops. Similar enhancement in the low-momentum region is observed in the CDB ratio spectra to pure Cu; see Fig. 4(b). The high-momentum region ($>15 \times 10^{-3}$ m_0c) is observed to be flat and increases toward pure Cu by increasing the annealing temperature (to 823 K).

The behavior of the low- and high-momentum regions can be quantified on the basis of S and W parameters. The S and W parameters are defined as the ratio of low-momentum ($|p_L| < 5 \times 10^{-3}$ m_0c) and high-momentum (15×10^{-3} $m_0c < |p_L| < 25 \times 10^{-3}$ m_0c) regions of the Doppler broadening spectra to the total region, respectively. The dependence of the S and W parameters as a function of the annealing temperatures are presented in Figs. 5(a) and 5(c), respectively. The increase of the annealing temperature causes a decrease of the S parameter (low-momentum contribution) as a consequence of dissociation of vacancy complexes. This defines the first recovery stage at about 723 K. The W parameter exhibits an increase and then a decrease by increasing the annealing temperature, with a peak value at about 823 K. Its increase occurs due to dissociation of vacancies from the vacancy-copper clusters resulting in the positron confinement in defect-free Cu precipitates.[14] The decrease of the W parameter is attributed to dissolution of Cu precipitates and defines the second recovery stage at about 923 K.

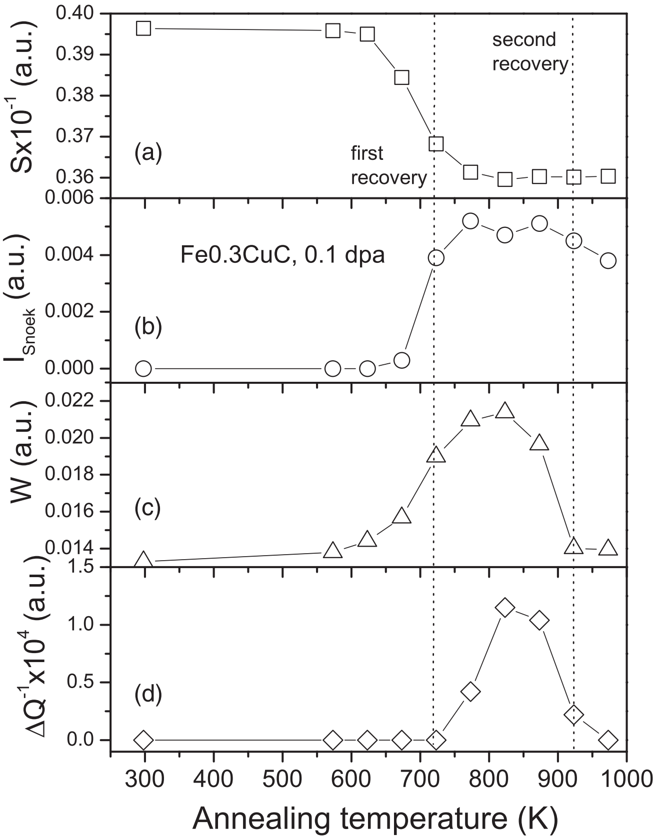

FIG. 5. Postirradiation annealing behavior of (a) the S parameter, (b) the intensity of the Snoek peak, (c) the W parameter, and (d) the magnitude of phase transition discontinuity.

The comparison of the results obtained by the IF and PAS experiments is shown in Fig. 5. The intensity of the Snoek peak and the magnitude of discontinuity, defined as $\Delta Q^{-1} = Q^{-1}(110\text{ K})–Q^{-1}(135\text{ K})$, as a function of the annealing temperatures are presented in Figs. 5(b) and 5(d), respectively. Interestingly, the intensity increase of the Snoek peak with the annealing temperature occurs in the same temperature interval where the S parameter decreases; see Figs. 5(a) and 5(b). This indicates that the appearance of Snoek peak can be correlated with the first recovery stage and that the dissociation of vacancies from copper-vacancy complexes at 723 K affects the carbon distribution in the lattice. Namely the dissolution/dissociation of vacancy-carbon clusters during the first recovery stage brings the carbon back to the iron lattice. These results reveal an additional complexity in the aggregation of vacancies, copper, and carbon atoms during neutron irradiation. Due to neutron irradiation the supersaturation of vacancies occurs, enabling easy formation of vacancy-copper complexes. It is plausible that such complexes, which are mobile, end up clustering with immobile C-vacancy complexes, giving rise to Cu-C-vacancy complexes. The fact that the CDB ratio spectra to pure Cu are flat in the high-momentum region [see Fig. 4(b)] indicates that the positron trapping sites are mostly covered with Cu atoms. This excludes the possibility for the existence of Cu free vacancy-C complexes in the material. In the following, the stability and dissociation of small Cu-C-vacancy complexes are analyzed by means of *ab initio* calculations.

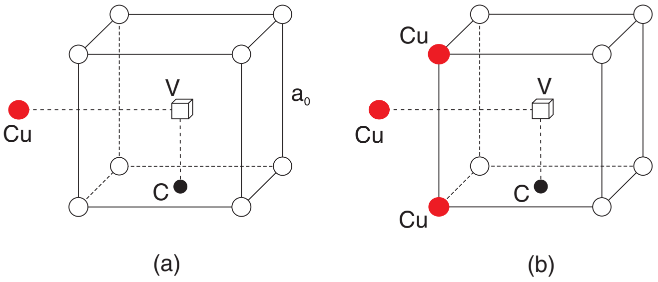

FIG. 6. (Color online) Atomic structure of copper-vacancy(V)-carbon (a) and 3Cu-V-C (b) complexes in bcc-Fe.

From earlier DFT calculations it is known that the Cu-V complex acquires the maximum binding energy (0.26 eV) if the two species are located as first nearest neighbors.[36] The most optimum configuration for a vacancy-carbon complex is realized for carbon in the octahedral configuration placed at $a_0/2$ distance from a vacancy. We find the corresponding binding energy E_b to be 0.65 eV. In the same configuration, C-Cu complex exhibits repulsive interaction with a binding energy of −0.42 eV. The repulsion vanishes with increasing distance between C and Cu. The most energetically favorable C-Cu-vacancy complex is shown in Fig. 6(a), for which the carbon and copper atoms are as far as $\sqrt{10}a_0/2$. The total binding energy of this complex is 0.83 eV, which means that coalescence of C, Cu, and vacancy into one cluster is an energetically favorable reaction. This result supports the experimental observation of the existence of Cu-C-vacancy clusters.

In order to calculate the dissociation energy (E_d), taken to be a sum of binding and migration energy, one needs to compute the partial binding energy of carbon with the vacancy-Cu complex. Note that Cu atom cannot migrate away from the complex without a transporting point defect, while the dissociation of a vacancy from this complex would result in the formation of weakly interacting Cu-carbon complex [because of a large distance between them, see Fig. 6(a)]. Hence, $E_b(\text{V-CuC}) \approx 0.83$ eV and $E_d(\text{V-CuC}) = 1.48$ eV, while $E_b(\text{C-VCu}) = 0.68$ eV and $E_d(\text{C-VCu}) = 1.57$ eV, which are obtained by taking the migration energy for a vacancy and carbon to be 0.65 and 0.89 eV, following available DFT data.[17,32] Thus, coalescence of carbon to a Cu-vacancy cluster increases not only the binding energy but also the dissociation energy. The dissociation of the Cu-C-vacancy cluster, via emission of C and/or vacancy, is equally probable process. This is in very good agreement with the experiment which shows that dissolution of vacancy clusters and free carbon appearance occur at the same temperature interval, e.g., at the first annealing stage.

In addition, the influence of carbon on multiple Cu-vacancy clusters is considered by analyzing the 3Cu-C-vacancy complex. The most favorable configuration for such a cluster is shown in Fig. 6(b). Carbon remains in the closest octahedral position, while two additional Cu atoms are added as first nearest neighbors to a vacancy. The total binding energy of this cluster is 1.78 eV, whereas the corresponding total binding energy without carbon is only 0.75 eV. The partial binding energy for carbon and vacancy is calculated to be 1.98 and 0.73 eV, which implies that the dissociation of such Cu-rich clusters occurs via emission of the carbon atoms, first, and then by the evaporation of vacancies. The dissociation energy for carbon in this case is 1.62 eV. However, once carbon is emitted from the cluster, the complex will break apart immediately since the dislocation energy for vacancy in the 3Cu-vacancy complex is only 1.2 eV. This additionally reinforces our previous conclusion that rearrangement of carbon and evaporation of vacancies from copper-rich clusters occurs simultaneously.

The change in IF coefficient, e.g., the magnitude of discontinuity as a function of the annealing temperature is presented in Fig. 5(d). The behavior of the IF discontinuity related to the phase transition at 122 K resembles the behavior of the W parameter; see Fig. 5(b). The ΔQ^{-1} exhibits an increase and then a decrease by increasing the annealing temperature, with a peak value at about 823 K. This finding suggests that the dissolution of vacancies from vacancy-copper(-carbon) clusters is accompanied by the subsequent full crystallization of Cu precipitates. It is indeed plausible that in neutron-irradiated Fe-Cu the large vacancy concentration prevents the formation of copper precipitate crystalline lattice. Thus, the neutron irradiated alloys, as well as the alloys that are annealed at temperatures lower than the first recovery stage, do not exhibit the structural phase transition at 122 K. This is in strong contrast with thermally aged Fe-1 wt. % Cu alloys, where the 122 K phase transition and crystalline Cu precipitates are already formed at an early precipitation stage.[22] At the first recovery stage annealing of vacancies occurs, resulting in the precipitates crystallization. This is manifested by the appearance of low-temperature phase transition in the IF spectra. By increasing the annealing temperature, the magnitude of the discontinuity increases due to the increase of the effective precipitate volume that crystallizes. It seems, however, that the onset of IF discontinuity occurs at temperatures slightly above the first recovery stage (of about 50 K). This could be either the consequence of measurement sensitivity or an indication of the existence of an intermediate state of copper precipitate (this requires further study). At the peak, the magnitude of IF discontinuity $\Delta Q^{-1} \sim 1.5 \times 10^{-4}$ [see Fig. 5(d)] is, roughly speaking, 3 times smaller than the ΔQ^{-1} saturation value obtained in thermally aged Fe-1 wt. % Cu alloys.[22] This result nicely correlates with the difference in copper concentrations in these two alloys. Further increase of the annealing temperature causes the decrease and disappearance of the ΔQ^{-1}, as a result of the second annealing stage at about 923 K which corresponds to the dissolution of copper precipitates.[14]

In copper-rich RPV steels, the irradiation-induced copper nanoclusters are expected to be more complex. Typically, in addition to forming complexes with vacancies and carbon, the copper clusters occur in synergy with other solute elements. The studies of these, by IF and PAS techniques, are underway.

V. CONCLUSION

In this study, we performed the internal friction and positron annihilation experiments of postirradiation annealed Fe-0.3 wt. % Cu-C alloys. We found that irradiation-mediated

Cu precipitation causes the formation of complex carbon-vacancy-copper clusters. These results are rationalized on the basis of *ab initio* calculations. The latter shows that the formation of small Cu-C-vacancy clusters is an energetically favorable reaction and that their dissociation occurs by simultaneous emission of vacancy and the carbon atoms. The cluster structure prevents formation of Cu precipitate crystalline structure. When vacancies and carbon atoms are removed by thermal annealing process at temperatures between the first and second recovery stages, the Cu precipitates do crystalize.

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