In Situ TEM Observation and MD Simulation of Frank Partial Dislocation Climbing in Al–Cu Alloy

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In situ electron irradiation using high-resolution transmission electron microscopy (HRTEM) was performed to visualize the Frank loop evolution in aluminum–copper (Al–Cu) alloy with an atomic-scale spatial resolution of 0.12 nm. The *in situ* HRTEM observation along the [110] direction of the FCC-Al lattice, Frank partial dislocation bounding an intrinsic stacking fault exhibited an asymmetrical climb along the (112) direction opposed to those in the reference pure Al under an electron irradiation, with a corresponding displacement-per-atom rate of 0.055–0.120 dpa/s in a high vacuum (1.2×10^{-5} Pa). We performed theoretical calculations to simulate the asymmetrical climb of the dislocation with Burgers vector *b* of 1/3(111). The Cu–Cu bonding in Guinier–Preston zones was described as a possible pinning site of the dislocation climb by molecular dynamics simulation. [doi:10.2320/matertrans.MT-M2021233]

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1. Introduction

In situ transmission electron microscopy (*in situ* TEM) helps visualize the microstructural evolution in the face centered cubic (FCC) lattice of aluminum (Al), under ion irradiation^{1,2)} and stress applications,³⁾ in real space and in nanometer scale. In the past 50 years, *in situ* TEM under an energetic electron beam irradiation has attracted particular interest. First, point defect clusters (Frank loops) were discovered in the Al lattice during a 1,000 kV high-voltage electron microscope (HVEM) observation in 1968.⁴⁾ The Frank loops introduced in pure aluminum by HVEM are normally interstitial types as demonstrated by Kiritani *et al.*⁵⁾ After discovering the point defect cluster in the FCC-Al lattice, multiple *in situ* TEM characterizations were performed with acceleration voltages above 400 kV to achieve a spatial resolution of 1 nm from thick samples, thus avoiding the surface effect.^{6,7)} Vacancy type Frank loops were also reported by Yang *et al.* in 1976.⁸⁾ These historical studies thereby increased our understanding of microstructural evolution and its dependence on temperature and irradiation rates of pure Al.

In contrast, high-resolution transmission electron microscopy (HRTEM) with a reasonable acceleration voltage of 200 kV has the advantage of being easily combined with aberration correctors,⁹⁾ chemical composition analysis and special sample holders. Idrissi *et al.* identified an intrinsic dislocation loop (Frank loop) induced by Ga ion irradiation at the atomic scale using aberration-corrected transmission electron microscopy (AC-TEM).¹⁾ Li *et al.* first achieved the *in situ* HRTEM of aluminum–zinc (Al–Zn) alloys and reported about interaction between Frank loops and precipitates in 2017.¹⁰⁾ Recently, *in situ* HRTEM tensile tests with the same FCC structure, such as copper and nickel in addition to Al, have also been reported.^{11–13)}

Hence, in this study, we applied the *in situ* HRTEM with 200 kV AC-TEM to aluminum–copper (Al–Cu) alloys. By comparing Frank loop behavior in pure Al and Al–Cu alloys, we attempted to visualize the pinning effect of a coherent precipitate, for example, Guinier–Preston (GP) zones,^{14–16)} on the climbing of the Frank partial dislocations. To visualize the pinning effect of the Cu–Cu bond (substitutional impurity) molecular dynamics (MD) simulations were also performed.

2. Experimental Procedures

Pure Al ($\Phi 3$ mm $\times$ 35 mm, purity 99.999%, The Nilaco Corp.) was cut into $\Phi 3$ -mm discs with thickness of 1 mm and then mechanically polished with abrasive paper discs (#600, #800, #1200 and #2000, Sankyo Rikagaku, Japan) and a dimple grinder (Model 656, Gatan Inc., USA). Thereafter, the Al discs were electrochemically polished using a twin-jet polishing machine (TenuPol-5, Struers.com, Denmark) with a mixture of 25% nitric acid and 75% methanol at a temperature below 0°C, and the applied potential of 10–12 V.

The commercially available Al–Cu alloy ($\Phi 3$ mm $\times$ 35 mm, Order No. 572684, Cu concentration; 1.7%, The Nilaco Corp., Japan) was solution-treated at 833 K for 1 h and quenched in water. The initial chemical composition of the Al–Cu alloy is shown in Table 1. The quenched Al–Cu alloy was cut into $\Phi 3$ -mm discs. Subsequently, the discs were mechanically ground to thicknesses of 75–95 μ m. Thin-film samples (approximately 20 nm thick) were prepared for *in situ* HRTEM observation using an Ar ion milling

Table 1 Composition of the Al–Cu alloy ($\Phi 3$ mm $\times$ 35 mm, Order No. 572684, Cu concentration; 1.7 at%).

Chemical composition [at. %]								
Si	Fe	Cu	Mn	Mg	Cr	Zn	Ti	Al
0.590	0.120	1.700	0.300	0.800	0.005	0.017	0.011	Bal.

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technique. The milling voltages were 5 kV for 8 hours; 4, 3, 2, 1 and 0.5 kV for 15 min each and 0.3 kV for 30 minutes. The milling angle was maintained at $\pm 4^\circ$ for all voltages. The two kinds of thin films fabricated for *in situ* TEM observation are shown as the Al-ref and the Al-1.7Cu samples.

In situ HRTEM was performed on a spherical aberration-corrected transmission electron microscope (ARM 200 F, JEOL Ltd., Japan) operated at 200 kV, the samples were observed from the $[110]$ axis of the FCC-Al lattice (close-packed direction). The microstructure evolution was recorded as a movie file using a TV-rate CCD camera (Orios SC 200TM, Gatan Inc., U.S.) with 20 frames per second. The chemical composition was evaluated by energy dispersive X-ray (EDX) spectroscopy in the high-angle annular dark-field scanning TEM (HAADF-STEM) mode.

The LAMMPS software suite was used for the MD calculation.¹⁷⁾ The original size of the MD simulation box was approximately $11 \times 23 \times 16 \text{ nm}^3$ and comprised of 256,000 atoms. The angular-dependent potential developed by Apostol and Mishin,¹⁸⁾ which is a generalization of the embedded-atom method, was applied to calculate the inter-atomic forces in the MD simulation model. The OVITO visualization tool,¹⁹⁾ was used to evaluate the simulation results.

3. Results and Discussion

Figures 1(a) and (b) show HAADF-STEM images obtained from the Al-1.7Cu sample along the incident axis

Fig. 1 HAADF-STEM image of the Al-1.7Cu sample in (a) thin and (b) thick regions; (c) EDX spectrum of the Al-1.7Cu sample.

$B = [110]$ at thin and thick areas, respectively.²⁰⁾ Figure 1(c) shows the EDX spectrum recorded at the thick area. The Cu concentration of the Al-1.7Cu sample calculated from the spectrum with background noise subtraction was $1.57 \pm 0.02 \text{ at\%}$. It was clarified from the HAADF-STEM images and EDX measurements that the contrast of the GP zone, which was reported in previous studies,^{21–23)} was not observed in the thin or the thick areas of the present Al-1.7Cu sample. This implies that Cu precipitates (including GP zones) in the commercial Al-1.7Cu alloy sample were successfully dissolved in the thermal treatment.

3.1 *In situ* TEM observations of Frank loop evolution in pure Al and Al-1.7Cu alloy samples

In situ TEM observations of the Al-1.7Cu sample are presented in Fig. 2. Figures 2(a)–(c) show HRTEM images captured from a TV rate movie file at 62, 124 and 248 s. The original movie file is available at <http://wani.imr.tohoku.ac.jp/MaterTrans2021.html>. The arrow (i) in the optical diffraction pattern in Fig. 2(b) shows the reflection vector corresponding to $\{1\bar{1}3\}$ planes of the FCC-Al lattice with a d-spacing of 0.12 nm.

Capture times of 62, 124 and 248 s correspond to the total irradiation times of 462, 524 and 648 s, respectively, from the starting point (gun valve opening) of 200 keV electron irradiation at RT. During electron irradiation, we discovered the growth of a Frank loop on increasing of the 200 keV electron dose. Along an electron incident angle of FCC-Al $[110]$, an ‘abcababc’ of stacking fault (SF) was visualized within the Frank loop in the Al-Cu alloy with atomic scale resolution of AC-TEM, as shown in Fig. 2(d). Figure 2(e) is a schematic diagram describing the intrinsic SF bounded by the vacancy-type Frank partial dislocation with Burgers vector $b = 1/3\langle 111 \rangle$ corresponding to the experimental TEM image in Fig. 2(d). The climb of the partial dislocation at the edge of the SF perfectly explains the increase in the SF in the present *in situ* HRTEM observation as described in Figs. 2(a)–(c). Direction of the climb was estimates to be in the $[1\bar{1}2]$ direction of the FCC-Al lattice. We believe that the vacancy clustering on the $\{111\}$ planes of the FCC-Al lattice is the driving force for the same. It can be considered that the increase in the total irradiation time causes a large number of vacancies to migrate to the Frank loop and contribute to the SF growth. The Frank loop is the sink site of interstitials as well as vacancies. The growth of the vacancy-type Frank partial dislocation means that absorption of vacancy is dominant in the present *in situ* HRTEM observation. Our findings on the *in situ* HRTEM observation of the Al-Cu alloy corresponded with those of the Al-Zn alloy in a previous study.¹⁰⁾ Except for the type and concentration of solute atoms, the *in situ* HRTEM observation of Al-Zn alloy proved useful. However, it is also well known that structural changes during *in situ* TEM observation strongly depend on microscope conditions, such as acceleration voltage, beam flux, and vacuum base pressure.

To further our understanding of the Frank loop evolution, the *in situ* HRTEM observation of the Al-ref sample was carefully carried out with the same beam flux of $3.7\text{--}8.6 \times 10^{20} \text{ e}^- \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$ in base pressure of $1.2 \times 10^{-5} \text{ Pa}$ using 200 kV AC-TEM. This beam flux can be converted to a

Fig. 2 (a)–(c) *In situ* HRTEM images of the Al–1.7Cu sample captured at 62, 124, and 248 s. Incident beam axis is $[110]$ of the FCC-Al lattice. The inset in (b) is an optical diffraction pattern; (d) is a high-magnification AC-TEM image taken at the edge of the planar defect. Lattice spacings of $d = 0.23$ nm and $d = 0.20$ nm for Al $(\bar{1}11)$ and (002) planes are indicated; (e) is a schematic diagram of the partial dislocation climb in the Al–1.7Cu sample.

displacement per atom (dpa) rate of 0.055–0.120 dpa/s using an atom displacement energy of 16 eV at 293 K.^{24,25)} In the case of pure Al, syntheses of Frank loops have been observed *in situ* in 1,000 kV TEM with 5.0×10^{-3} dpa/s,^{4,5,7,8)} 400 kV TEM with 3.7×10^{-4} and 3.7×10^{-3} dpa/s,⁶⁾ and 200 kV TEM with 5.0×10^{-3} to 1.2×10^{-1} dpa/s.^{26,27)}

Figure 3 shows the *in situ* HRTEM observation of the Al-ref sample. Figures 3(a)–(c) are HRTEM images captured at 90, 120 and 150 s from a TV rate movie file obtained from the Al-ref sample. The original movie file is available at <http://wani.imr.tohoku.ac.jp/MaterTrans2021.html>.

The Frank loop shown in Fig. 3(a) is evidence of the reproducibility of the present *in situ* HRTEM technique for electron irradiation testing of Al lattice defects. Additionally, the *in situ* HRTEM observation had successfully visualized the crystallographic symmetry of the vacancy type Frank loop evolution in the Al-ref sample. The details are showed in the schematic diagram in Fig. 3(d). First, a Frank loop was observed on (111) plane lying along the electron incident direction of $[110]$. When the Frank loop grow up and the size of the loop became nearly equal to the sample thickness of 10–20 nm, then a clear contrast corresponding to the intrinsic SF started to appear in the HRTEM image. At both sides of the intrinsic SF, partial dislocations with Burgers vector $\mathbf{b}$ of $1/3\langle 111 \rangle$ were visible. Because sides (i) and (ii) belong to

one Frank loop, the climb of sides (i) and (ii) should have an opposite relation to the climbing direction along $[1\bar{1}2]$. This is the crystallographically symmetrical growth of the Frank loop.

In addition, we discuss about contribution of interstitial Al atoms to understand why the vacancy type Frank loop was observed instead of the interstitial type Frank loop or double-loop.^{4,27)} Initial FCC-Al lattice is vacancy rich at RT; the thermal equilibrium vacancy concentration is $5.66 \times 10^{19}/\text{cm}^3$. Formation energy E_f and migration energy E_m of interstitial atom is 3.2 eV and 0.12 eV. In contrast ones of vacancy are just 0.67 eV and 0.62 eV. We thought that interstitial atom which are generated beyond the higher energy barrier of E_f can easily diffuse and disappear into top and bottom surfaces in ultra-thin samples for *in situ* HRTEM. Caused by vacancy supersaturation environment due to being sandwiched between surfaces spaced 20 nm apart, contribution of interstitial Al atoms on the growth of irradiation should be considerably lower than ones in previous HVEM observations using sample thicker than 500 nm.

However, actually even when the sample thickness is the ultra-thin for atomic resolution, we can enhance contribution of interstitial Al atoms by increasing the concentration of impurity atoms. The high sensitivity of interstitial atoms

Fig. 3 (a)–(c) *In situ* HRTEM images of the Al-ref sample captured at 60, 90 and 120 s. Incident beam axis is $[110]$ of the FCC-Al lattice. The inset in (a) is an optical diffraction pattern indicating reflection vectors of $(\bar{1}11)$, $(1\bar{1}1)$, and (002) ; (d) schematic diagram of the Frank loops in a 20 nm thin sample with plane and cross-sectional views along incident axis $B = [110]$.

clusters to impurities in the FCC-Al lattice has already been confirmed by HVEM observations by Shimomura *et al.*²⁸⁾ In the case of the Al–Cu alloys, substitutional Cu impurity is under-size element in Al matrix, and thus is expected to migrate together with interstitials. One can say that *in situ* HRTEM observations of the Al–1.7Cu sample visualizes behavior of such interstitial atoms, relatively, through the precipitation behavior of Cu precipitates and the stability of the vacancy type Frank loop.

The highlight of the present *in situ* HRTEM observation is the asymmetrical growth of the Frank loop observed in the Al–1.7Cu sample. As shown in Fig. 3, the *in situ* HRTEM of Al-ref achieved atomic-scale visualization of the symmetrical growth of the Frank loop. Figure 4(a) shows a HRTEM image of the Al–1.7Cu sample captured at 540 s after electron irradiation began. Diameters of Frank loop *A* in diameter and Frank loop *B* were 4.48 and 6.92 nm on the $\{111\}$ plane. In 100 s, loops *A* and *B* grew to 9.35 and 8.49 nm, respectively. During the growth process of the Frank loops, the edge dislocation on one side, indicated by the red color in Fig. 4(a)–(c), climbed stepwise. The edge dislocation on the other side (in blue) was stabilized and never climbed. A considerable strain contrast was observed between the two stable edge dislocations, as shown in Fig. 4(c). The strain contrast was maintained through the growth process of the Frank loops. In addition, the HRTEM interference pattern in region (i) always suggests a coherent crystal orientation with the $[110]$ FCC-Al lattice. Figure 4(d) shows the intensity line profiles obtained from regions (i) and (ii) in Fig. 4(c). The maximum intensity of profile (i) was almost same as that of

profile (ii), and their peak widths were 0.41 nm and 2.71 nm, respectively, which implies that the peak width of profile (i) was 6.6 times larger than that of profile (ii). These results indicate that there is a coherent object experiencing a large lattice strain in region (i), which provides a stronger strain contrast than the $1/3\langle 111 \rangle$ type partial dislocation. One reasonable explanation is the coherent precipitates on $\{100\}$, such as the GP zones, as shown in Fig. 4(e). The bonding length of Cu–Cu atoms is 0.26 nm, which is much shorter than that (0.29 nm) of Al–Al atoms. Coherent Cu precipitates can explain the strain contrast in the experimental HRTEM images during *in situ* electron irradiation of the Al–1.7Cu sample.

Figure 5 shows schematic diagrams for a simplified understanding of the effects of interstitials, vacancies, and Cu impurities on growth and shrinkage of flank loops. The Frank loop is the sink site of point defects such as interstitials and vacancies. Absorption of interstitials results in shrinkage of the vacancy type Frank loop. If the same number of interstitials as vacancies are absorbed into the Frank loops, the size remains unchanged. These are universal theory on irradiation defects in the Al–1.7Cu sample. In Fig. 4, the way of growth changed to be heterogeneous by addition of copper. In this study, we assume a heterogeneous structure as shown in Fig. 4(e). In this asymmetrical structure, Cu–Cu bonds are introduced into only side (ii) of the vacancy type Frank loop. The simplest structure consists of such Cu–Cu bonds that satisfies the crystallographic periodic boundary conditions is GP zone, which is calculated in the next section 3.2.

Fig. 4 *In situ* HRTEM images of the Al-1.7Cu sample after 10 min irradiation. (a)–(c) HRTEM images of the Al-1.7Cu sample captured at 0, 60, and 100 s (initial time 0 s is 540 s after electron irradiation began); (d) intensity line profiles obtained from regions (i) and (ii) in (c); (e) schematic diagram showing coherent Cu precipitate sandwiched between two Frank loops.

Fig. 5 (a) Schema of thickness of observation areas in the present *in situ* HRTEM and *in situ* HVEM. (b) Atomic-scale phenomena considered to be occurring in the Al-1.7Cu sample.

3.2 MD simulation of dislocation pinning at coherent precipitates

In this section, the GP zones (planar Cu precipitates: coherent) synthesized during *in situ* electron irradiation are suggested as obstacles on $\{100\}$ planes for $\{111\}$ edge dislocation movement.²¹⁾ Therefore, to investigate the interaction between GP zones and edge dislocations during electron irradiation, we calculated the dynamical behavior of the interaction via an MD simulation. For the MD simulation, which was based on the FCC-Al lattice, one (001) GP zone and one SF (Frank loop) on the $(1\bar{1}1)$ plane were initially prepared in three-dimensional space. To better identify the interaction process, the (001) GP zone is shown in blue and the $(1\bar{1}1)$ Frank loop, indicated in green are shown at the center of the MD simulation box in such common neighbor analysis (CNA) using the OVITO visualization tool.¹⁹⁾ FCC atoms are invisible in the CNA map.

To describe the climb of the edge dislocation, 0.001 tensile strain along the $[1\bar{1}0]$ direction was imposed on the MD simulation box, and the atomic positions in the box were relaxed. Note that the tensile deformation was associated with a stepwise compressive deformation along the x- and z-directions according to the Poisson's ratio of Al (0.33); Fig. 6(a) shows a snapshot corresponding to the 30th step of the lattice relaxation as a key point of the MD simulation.

The synthesis and growth of two edge dislocations ($\bar{1}11$) planes, at both sides of the SF, can be observed. One edge dislocation at side (i) is climbing along $[\bar{1}\bar{1}2]$ and the other side (ii) reaches the GP zone with a relative angle of 54.74° , as displayed in Fig. 6(a), showing considerable interaction. The supporting movie file showing relaxation process of the present MD simulation is available at <http://wani.imr.tohoku.ac.jp/MaterTrans2021MD.html>. Figures 6(b) and (c) are slice views of the MD simulation box at the crossing of the edge dislocation and GP zone along the $[1\bar{1}2]$ and $[1\bar{1}0]$ directions. The green line connecting atoms on the misfit strain field (blue spheres) can be considered a dislocation line. The dislocation line was bent significantly under the influence of the negative lattice strain field of the GP zone. The repulsive force was greatest in the red-circled area (Fig. 6(c)). As described in the slice images in Figs. 6(d)–(f), the lattice strain was perfectly relaxed when the GP zone was cut and the dislocation passed through. We iterated the deformation step until the edge dislocation was unpinned from the GP zone, where the tensile strain and stress were 0.033 and 2.27 GPa, respectively. The present MD simulation successfully defined the coherent Cu precipitate on (001) as having a shorter bonding length of 0.264, which hampers the climb of the $(1\bar{1}1)$ edge dislocation by the repulsive force between strain fields. This understanding can be extended to

Fig. 6 CNA maps of MD simulation results of the interaction between dislocations and a GP zone by OVITO. (a) Snapshot of key moments of the simulation; (b), (c) interaction regions of (a) along the $[1\bar{1}2]$ and $[1\bar{1}0]$ directions; (d)–(f) complete interaction process in the MD simulation. The coloring of atoms is based on common neighbor analysis method.

the GP zones on the crystallographically equivalent (100) and (010) planes. Similarly, general mixed dislocations can also be decomposed into independent edges and helical components in dislocation theory; therefore, the present inhibition effect of the strain field of coherent precipitates can be applied to a part of simple Al–Cu alloys. In this study, we focused on the coherent precipitates in commercial Al–1.7Cu (at%) alloy as an initial precipitation-hardening model of the 2xxx series, however, the building-up of supercells for MD simulation to match with precipitation hardening processes of the actual Al–Cu alloys would be challenging.^{14,15} Further, the *in situ* HRTEM observation as an experimental approach can be more widely applied to Al–Zn, Al–Cu–Zn, Cu–Be, Fe–Mo, Al–Ag and Al–Mg–Si alloys, when considering precipitation hardening.^{29–31} Atomic-scale visualization of typical defect structures and their evolution using the present *in situ* HRTEM will support modeling and simulation as demonstrated in this study.

4. Conclusions

In situ HRTEM with 200 kV AC-TEM was applied for compare Frank partial dislocation loops in pure Al and Al–Cu alloy (1.7% of Cu) in real-time. With a beam flux of $3.7\text{--}8.6 \times 10^{20} \text{ e}^- \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$ and base pressure of $1.2 \times 10^{-5} \text{ Pa}$, symmetrical/asymmetrical climbs along of $\langle 112 \rangle$ were successfully visualized with 0.12 nm resolution from $[110]$ direction of the FCC-Al lattice. The Frank loop was identified as the $1/3(111)$ vacancy type Frank loops in pure Al as well as the Al–Cu alloy by direct observation of the intrinsic SF. The asymmetrical dislocation climb observed in the Al–Cu alloy was especially, focused and an additional MD simulation was performed to evaluate the influence of the strong Cu–Cu bond of coherent Cu precipitates on the dislocation–precipitate interaction. The MD analysis of the dislocation–GP zone interaction was performed to understand the asymmetrical climb of the Frank loop as a trial.

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REFERENCES

- 1) H. Idrissi, S. Turner, M. Mitsuhashi, B. Wang, S. Hata, M. Coulombier, J.P. Raskin, T. Pardoen, G.V. Tendeloo and D. Scheyvers: *Microsc. Microanal.* **17** (2011) 983–990.
- 2) K. Hattar, D.C. Bufford and D.L. Bullar: *Nucl. Instrum. Methods Phys. Res. B* **338** (2014) 56–65.
- 3) S.H. Oh, M. Legros, D. Kiener and G. Dehm: *Nat. Mater.* **8** (2009) 95–100.
- 4) M.J. Makin: *Philos. Mag.* **18** (1968) 637–653.
- 5) M. Kiritani, N. Yoshida and H. Takata: *J. Phys. Soc. Jpn.* **36** (1974) 720–729.
- 6) S. Jitsukawa and K. Hojou: *J. Nucl. Mater.* **212** (1994) 221–225.
- 7) K. Shiraishi, A. Hishinuma, Y. Katano and T. Taoka: *J. Phys. Soc. Jpn.* **32** (1972) 964–971.
- 8) W.J. Yang, R.A. Dodd and G.L. Kulcinski: *J. Nucl. Mater.* **64** (1977) 157–166.
- 9) M. Haider, H. Rose, S. Uhlemann, E. Schwan, B. Kabius and K. Urban: *Ultramicroscopy* **75** (1998) 53–60.
- 10) S. Li, H. Luo, H. Wang, P. Xu, J. Luo, C. Liu and T. Zhang: *Crystals* **7** (2017) 375.
- 11) H.P. Anwar Ali and A. Budiman: *J. Mater. Res.* **34** (2019) 1449–1468.
- 12) V. Samaee, M. Dupraz, T. Pardoen, H.V. Swygenhoven, D. Schryvers and H. Idrissi: *Nat. Commun.* **12** (2021) 962.
- 13) K. Hattar, J. Han, M.T.A. Saif and L.M. Robertson: *J. Mater. Res.* **20** (2005) 1869–1877.
- 14) A. Guinier: *Nature* **142** (1938) 569–570.
- 15) G.D. Preston: *Proc. R. Soc. London Ser. A* **167** (1938) 526–538.
- 16) V. Gerold and H. Haberkorn: *Phys. Status Solidi B* **16** (1966) 675–684.
- 17) S. Plimpton: *J. Comput. Phys.* **117** (1995) 1–19.
- 18) F. Apostol and Y. Mishin: *Phys. Rev. B* **83** (2011) 054116.
- 19) A. Stukowski: *Model. Simul. Mater. Sci. Eng.* **18** (2010) 015012.
- 20) E. Abe: *Mater. Trans.* **44** (2003) 2035–2041.
- 21) T.J. Konno, M. Kawasaki and K. Hiraga: *Philos. Mag.* **81** (2001) 1713–1724.
- 22) L. Bourgeois, C. Dwyer, M. Weyland, J.F. Nie and B.C. Muddle: *Acta Mater.* **59** (2011) 7043–7050.
- 23) Z. Shen, Q. Ding, C. Liu, J. Wang, H. Tian, J. Li and Z. Zhang: *J. Mater. Sci. Technol.* **33** (2017) 1159–1164.
- 24) G.S. Was: The displacement of atoms, *Fundamentals of Radiation Materials Science: Metals and Alloys*, second ed., (Springer, Berlin, 2017) pp. 77–89.
- 25) N.T.H. Trung, H.S.M. Phuong, M.D. Starostenkov, V.V. Romanenko and V.A. Popov: *IOP Conf. Ser.: Mater. Sci. Eng.* **447** (2018) 012004.
- 26) A. Wolfenden: *Micron* **3** (1972) 51–61.
- 27) S. Yoshida and Y. Shimomura: *J. Phys. Soc. Jpn.* **18** (1963) 1590–1593.
- 28) Y. Shimomura and S. Kuwabara: *J. Phys. Soc. Jpn.* **42** (1977) 1221–1228.
- 29) W.M. Lee and M.A. Zikry: *Metall. Mater. Trans. A* **42** (2010) 1215–1221.
- 30) D.T. Casem and D.P. Dandekar: *J. Appl. Phys.* **111** (2012) 063508.
- 31) W.M. Lee and M.A. Zikry: *Int. J. Solids Struct.* **49** (2012) 3291–3300.