

Molecular dynamics simulation of microcrack healing in copper

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Abstract

The molecular dynamics method is used to simulate microcrack healing during heating or/and under compressive stress. A center microcrack in Cu crystal could be sealed under a compressive stress or by heating. The role of compressive stress and heating in crack healing was additive. During microcrack healing, dislocation generation and motion occurred. If there were pre-existed dislocations around the microcrack, the critical temperature or compressive stress necessary for microcrack healing would decrease, and the higher the number of dislocations, the lower the critical temperature or compressive stress. The critical temperature necessary for microcrack healing depended upon the orientation of crack plane. For example, the critical temperature of the crack along (001) plane was the lowest, i.e., 770 K. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The microcracks in ceramic [1–3], plexiglass [4] and ice [5] could be healed through atom diffusion during heating. Microcrack in metal materials can also be healed. For example for hot-rolled Inconel 600 alloy, microcracks initiating early at the grain boundary were closed during heating over 870°C with a large compressive stress by moving grain boundaries because of recrystallization [6]. For Cu30Fe duplex alloy, microcracks forming early during rolling at room temperature could be closed after rolling exceeded 30% [7]. For 20 MnMo steel, microcracks disappeared during hot deformation

[8]. In situ TEM observations showed that for metal materials, whether ductile or brittle, dislocation emission and motion occurred before and during crack initiation or/and propagation [9–11]. Therefore, the resistance for crack propagation is $2\gamma + \gamma_p$, where γ is the surface energy and γ_p the plastic work. What remains to be elucidated is whether dislocation emission and motion are involved in microcrack closure or healing; or plastic deformation is also involved in the resistance required for microcrack healing?

Dislocation emission and crack propagation can be simulated by molecular dynamics method [12–14]. In the present paper, the molecular dynamics method is used to simulate microcrack healing during pressing or heating, and to exhibit the role of the plastic deformation in microcrack healing.

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2. Computation procedure

Copper was chosen as the simulated material. The inter-atomic potential used here is the N-body potential proposed by Finnis and Sinclair [15] according to the embedded atom method (EAM) and constructed by Ackland et al. [16]. The inner atoms follow law of Newton, and the leapfrog algorithm [17] is applied to calculate positions and velocities of atoms. The initial velocity is the Maxwell–Boltzmann distribution corresponding to a given temperature. The system temperature is maintained at a constant value by scaling the atom velocities during the simulations.

The x axis is along the extension line of the center crack, the y along the normal of the crack plane, and the z along the $[1\ 1\ \bar{2}]$ direction. The inclination angle θ between the $(1\ 1\ 1)$ slip plane and the crack plane changes from 0° to 90° , and in general, is set to be 70° , as shown in Fig. 1(a), where a_0 is the lattice constant, the length of the crystal along the x axis direction is $45 \times \sqrt{2}/2a_0$. The width along the y axis direction is $25 \times \sqrt{3}a_0$, and the thickness along the z axis direction is $\sqrt{2}/2a_0$. The number of atoms used here is about 6000. The length of the center crack is $2a = 3.6$ nm, and width is 0.6 nm, which is larger than the potential cutoff distance, which is 0.44 nm.

During the heating, a fixed boundary condition is used in the x and y directions. That is, the locations of the boundary atoms are remained unchanged during the whole calculation process. During loading and heating under a compressive stress, the displacement boundary condition is used in the x and y directions. That is, the boundary atoms move according to the plane strain linear elastic displacement field for a cracked solid [18]. Along the z direction, a six layer periodic representation is applied in all simulation.

The edge-cracked crystal is easy to emit dislocation during mode I loading [12–14] but cannot be closed. For the center-cracked crystal, the situation is quite opposite. In order to generate dislocations in the center-cracked crystal, the edge-cracked crystal is to be used to emit dislocations under mode I loading, and then the atomic configuration in the area containing the dislocations, which contains 24×24 rows atoms, is copied to

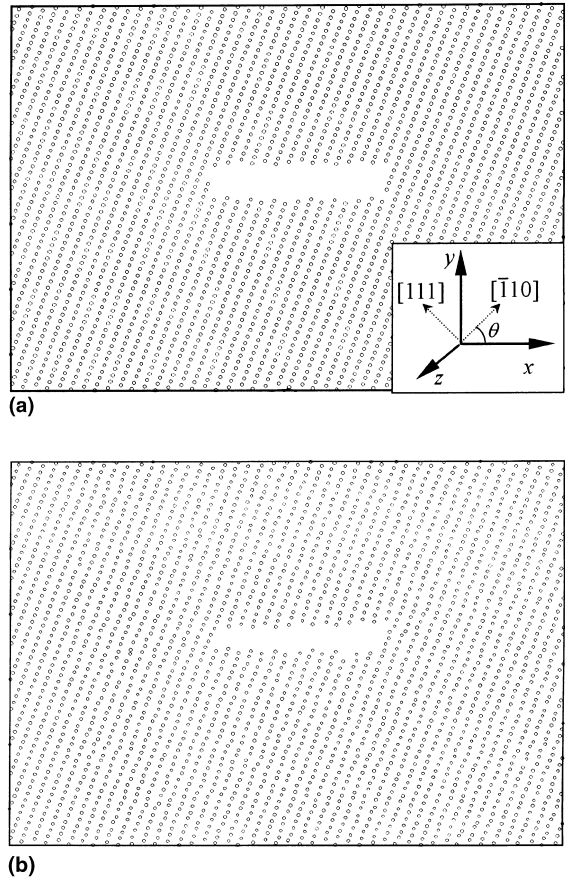


Fig. 1. The atomic configuration obtained by relaxing at 40 K (a) and at 700 K (b).

the center-cracked crystal. During coping, the relative displacements between boundary atoms of the area containing the dislocations and their nearest atoms in the edge-cracked crystal are the same as those in the center-cracked crystal.

3. Results and discussion

3.1. Crack healing by heating

The inclination angle θ between the crack plane and the $(1\ 1\ 1)$ slip plane is 70° . After the center crack is formed, the configuration is relaxed at 40 K, which is near to 0 K, until reaching

equilibrium, as shown in Fig. 1(a). The temperature is chosen to be 600, 650, 700, 750 and 800 K, respectively, and maintained at a constant during relaxation. The time step is 7.5×10^{-4} ps. Simulations show that when temperature is maintained at 600, 650 and 700 K, the center crack cannot close after relaxing for 50 ps, which is a relatively long time, as shown in Fig. 1(b). If the temperature is maintained at 750 K, the crack begins to heal after relaxing for 3 ps along with generating dislocations, as shown in Fig. 2(a). After 7.5 ps, the crack is approximately healed, but a void V and some dislocations as B, C , and D are left, as shown in Fig. 2(b). The void does not disappear after relaxing for 50 ps at 750 K. At 800 K, the crack is closed completely after relaxing for 9 ps,

and some dislocations as A, B, C, D, E, F and G but no void are left, as shown in Fig. 2(c).

3.2. Crack healing by compressive stress

Remaining the temperature at 40 K, a compressive stress σ perpendicular to the crack plane is applied with a loading rate of 0.13 GPa/ps. When the compressive stress increases to $\sigma = 7.26$ GPa, the crack heals to some extent, but a void and some dislocations are left, as shown in Fig. 3(a). When the compressive stress is increased to $\sigma = 13.2$ GPa, the crack closes completely, and some dislocations but no void remain in the crystal, as shown in Fig. 3(b).

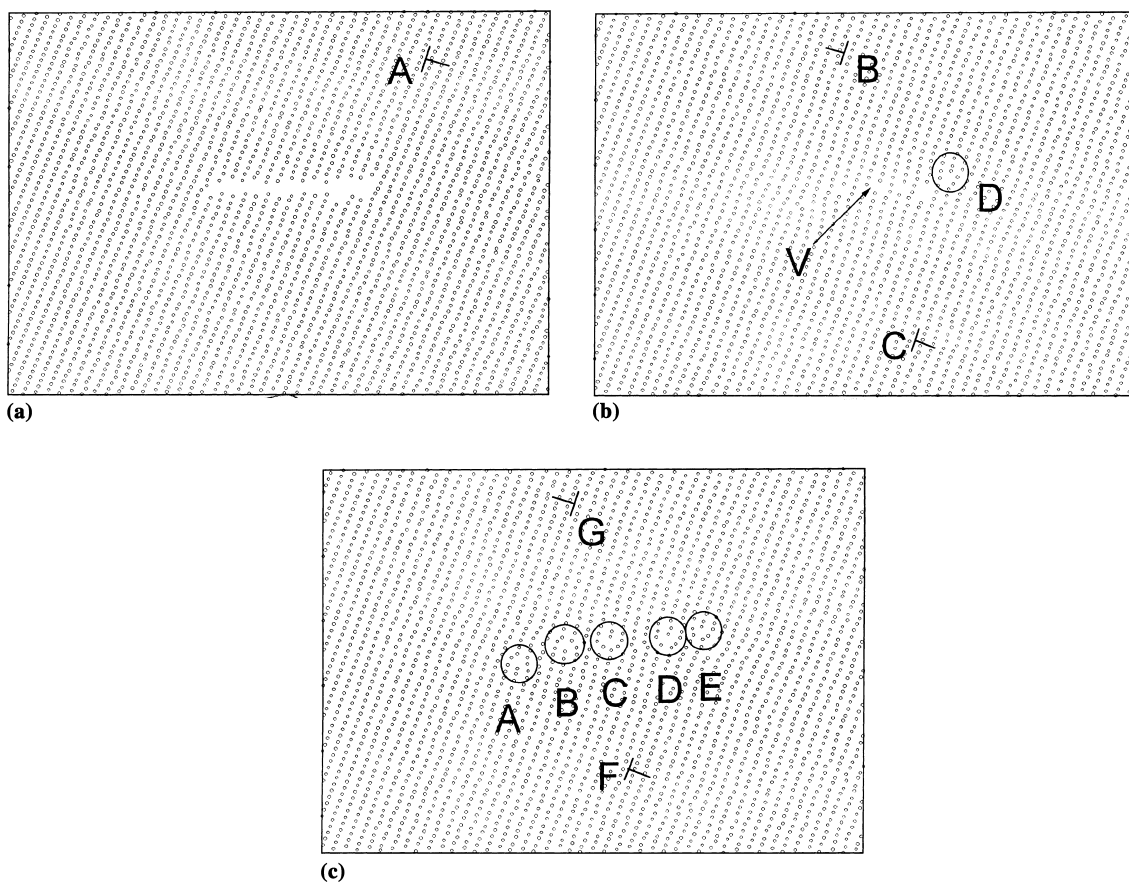
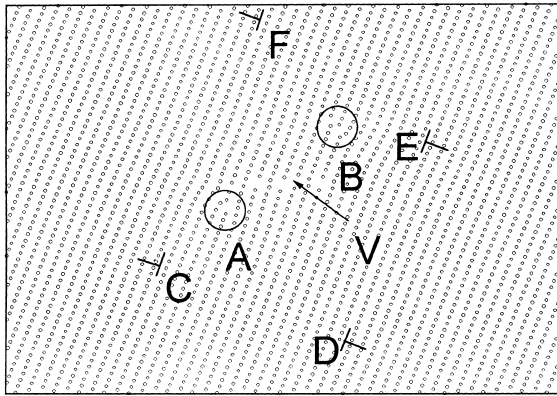
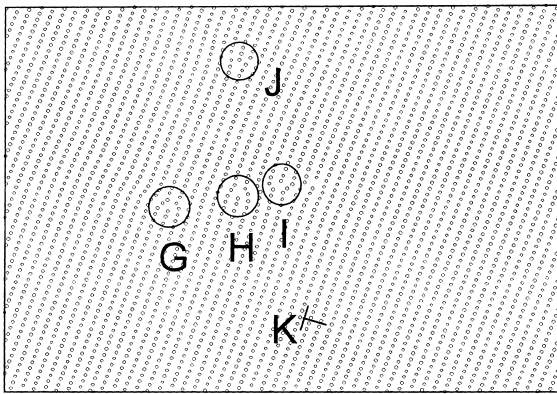


Fig. 2. Crack healing process. After relaxing for 3 ps (a), 7.5 ps (b) at 750 K, and for 9 ps at 800 K (c). A to G are dislocations and V void.



(a)



(b)

Fig. 3. Crack healing under compressive stress of 7.26 GPa (a) and 13.2 GPa (b) at 0 K. *A* to *K* are dislocations, *V* void.

3.3. Crack healing during heating under compressive stress

Simulations show that the critical compressive stress and critical temperature necessary for crack healing are $\sigma_c = 13.2$ GPa and $T_c = 800$ K, respectively. If compressive stress $\sigma = 3.96$ GPa is applied and temperature is maintained at 600 K, the crack is closed completely after relaxing for 11.25 ps and some dislocations are left, as shown in Fig. 4. Therefore, the applied compressive stress of 3.96 GPa can decrease the critical temperature necessary for crack healing from 800 to 600 K. Fig. 4 also indicates that increasing temperature from 40 to 600 K can reduce the critical compressive stress necessary for crack healing from

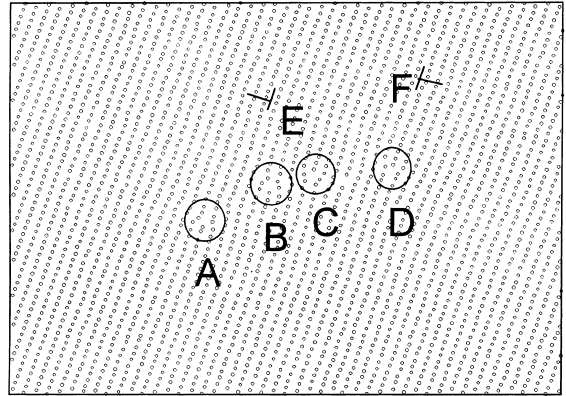


Fig. 4. Crack healing at 600 K under $\sigma = 3.96$ GPa, *A* to *D* are Frank dislocations, *E* and *F* Shockley dislocations.

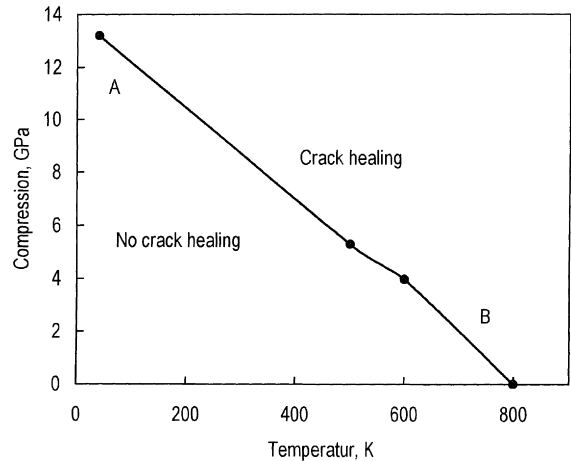


Fig. 5. The regions of crack healing and no crack healing in the coordinate system of temperature and compressive stress.

13.2 to 3.96 GPa. If the compressive stress is 5.28 GPa, the temperature for crack healing is 500 K. These results indicate that the role of compressive stress and heating in crack healing is additive. Fig. 5 shows that the crack healing can occur above the curve *AB*, and no crack healing under the curve *AB*.

3.4. Effect of orientation of crack plane on crack healing

If the crack plane is along the (111) slip plane ($\theta = 0$), the critical temperature necessary for

crack healing is 850 K instead of 800 K, as shown in Fig. 6(a). Crack healing at 850 K is also accompanied with the generation and movement of dislocations.

If the crack plane is along (001) plane ($\theta = 54.7^\circ$), the critical temperature of crack healing is 770 K, as shown in Fig. 6(b). When the crack plane is along ($\bar{1}10$) plane ($\theta = 90^\circ$), the critical temperature of crack healing is 790 K, as shown in Fig. 6(c).

3.5. Effect of dislocation on crack healing

For the edge-cracked crystal, a tensile stress perpendicular to the crack plane is applied with a loading rate of 0.079 GPa/ps. When $\sigma_1 = 3.95$ GPa

corresponding to 10 000 time steps, the first Shockley dislocation is emitted from the crack tip, and when $\sigma_1 = 4.74$ GPa corresponding to $K_I = 0.6$ MPam^{1/2}, two Shockley dislocations are emitted from the tip of the edge crack, as shown in Fig. 7(a). The atomic configuration of the edge-cracked crystal in area *A*, which contains the two dislocations, is copied to the center-cracked crystal, as shown in Fig. 7(b).

For the center-cracked crystal containing no dislocation, the critical temperature for crack healing is 800 K, as shown in Fig. 2(c). However, when the center-cracked crystal containing two Shockley dislocations is maintained at 650 K, the crack begins to heal after 2500 time steps, at the same time, the pre-existing dislocations have disappeared and some new dislocations have

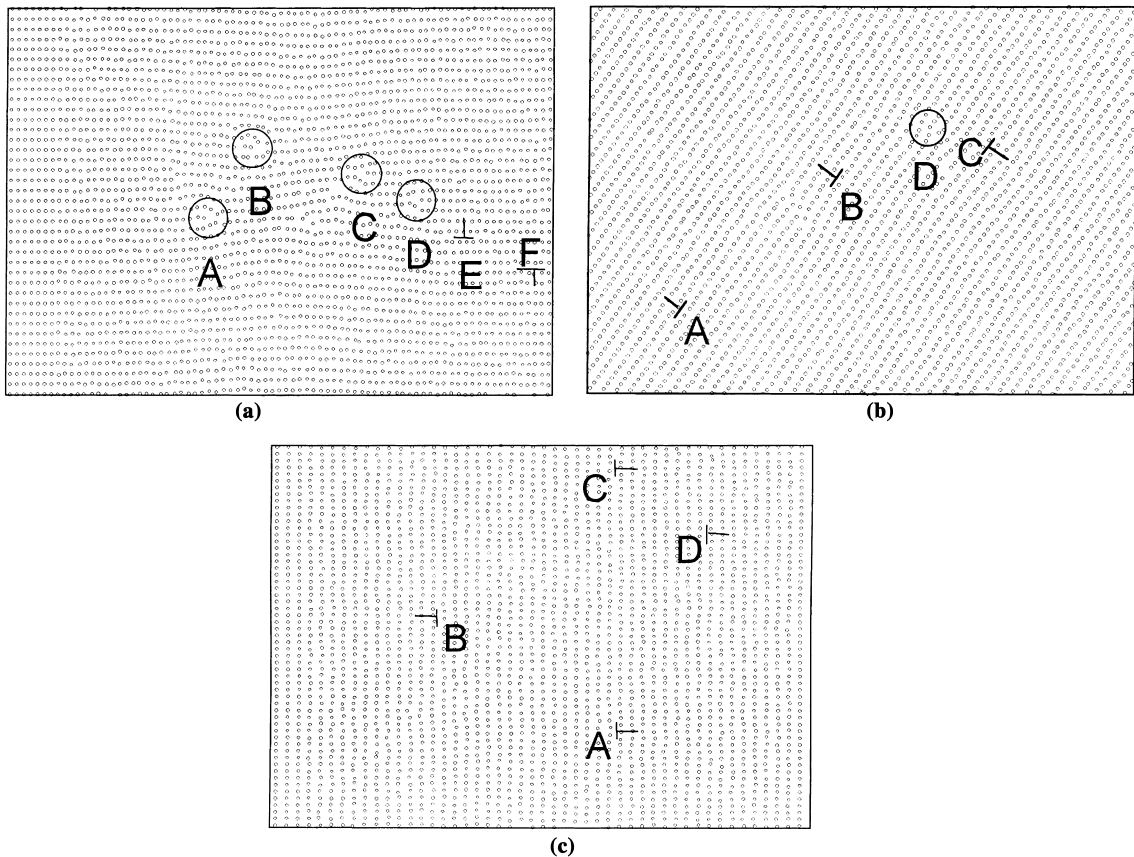


Fig. 6. Healing of the crack along (111) plane at 850 K (a), (001) plane at 770 K (b) and ($\bar{1}10$) plane at 790 K (c).

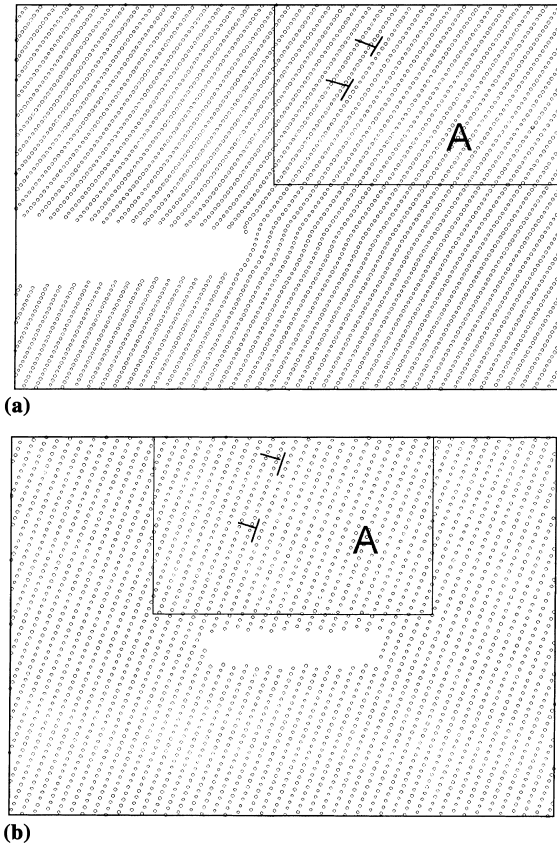


Fig. 7. The atomic configuration containing two dislocations, (a) edge crack, (b) center crack.

appeared. After relaxing at 650 K for 10 000 time steps, the crack is closed completely and some new dislocations form, as shown in Fig. 8(a). This shows that two pre-existing dislocations can reduce the critical temperature necessary for crack healing from 800 to 650 K. For the center-cracked crystal without dislocations, the critical compressive stress necessary for crack healing at 40 K is $\sigma = 13.2$ GPa, as shown in Fig. 3(b). If there are two pre-existing dislocations, the crack will be closed completely under a compressive stress $\sigma = 9.9$ GPa at 40 K, as shown in Fig. 8(b). This indicates that two pre-existing dislocations can decrease the critical compressive stress for crack healing from 13.2 to 9.9 GPa. In a word, pre-existed dislocations can promote crack healing. If the atomic configuration in the

area *A* shown in Fig. 7(a) is copied twice to the center-cracked crystal, there are four pre-existing dislocations. At 500 K, the crack has been completely closed after relaxing for 6500 time steps and some dislocations are generated, as shown in Fig. 8(c). Therefore, pre-existing dislocation can decrease the critical temperature for crack healing and the higher the number of the pre-existing dislocations, the lower the critical temperature for crack healing.

Applied compressive stress σ can cause crack healing, as shown in Fig. 3, therefore, the elastic energy $\sigma^2 \pi a(1 - \nu^2)/E$ is a driving force for crack healing. On the other hand, heating can cause crack healing, hence thermal energy is also the driving force for crack healing. Fig. 4 indicates that the compressive stress can decrease the critical temperature for crack healing, and increasing the temperature can reduce the critical compressive stress for crack healing. This shows that the two driving forces are additive, as shown in Fig. 5. Fig. 8 shows that pre-existing dislocations could reduce the critical temperature or the critical compressive stress for crack healing. Maybe the pre-existing dislocations can reduce the resistance of crack healing.

4. Conclusions

1. Compressive stress or heating can cause crack healing up and their role is additive.
2. Crack healing is accompanied with the generation and movement of dislocations.
3. The critical temperature of crack healing is related with the orientation of crack plane.
4. Pre-existing dislocations can reduce the critical temperature necessary for crack healing.

Acknowledgements

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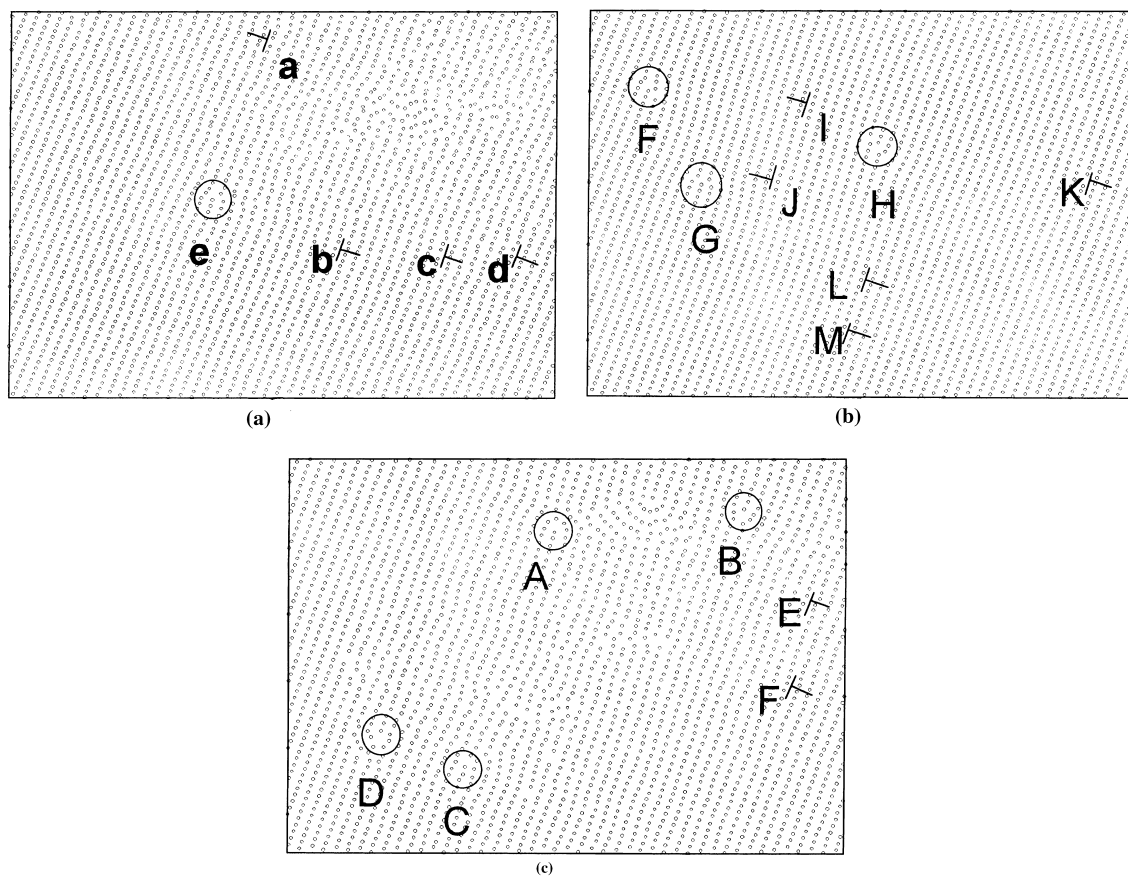


Fig. 8. Crack healing for the crystal containing two dislocations at 650 K (a), at 0 K but under a compressive stress of 9.9 GPa (b), and containing four dislocations at 500 K (c).

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