Movies of Mode-I Fracture Processes of the Iron Crystals by Molecular-Dynamics Simulations

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Abstract

Atomistic processes of the mode-I fracture of α-iron are demonstrated by movies, which show that the bcc-Fe is intrinsically brittle at lower temperatures and ductile at higher temperatures. The fracture of α-iron at lower temperatures is shown to take place by propagation of a crack along a specific plane of the iron crystals. On the contrary, the fracture of the crystals at higher temperatures is shown to occur by plastic deformation. Moreover an icosahedral structure is observed to form at the neck of the specimen shortly before an overall rupture in the high temperature deformation process.

1. Introduction

The integration of numerical calculations, data analysis, and their visualization may allow one to derive a new concept or a novel discovery in the field of materials science. In this study, we made molecular-dynamics simulations of the fracture process of α-iron crystals. The resultant huge amount of data is transformed into pictures in movies which enables us vividly observe the dynamic processes of extremely small regions in crystals and also enable us to obtain some new information relevant to the present subject.

2. Method of Simulation and Visualization

Specimen of a-iron crystal with bcc structure and with an initially introduced mode-I crack (see Fig. 1) are constructed using the Johnson's interatomic potential proposed for Fe-C system[1]. This potential can well reproduce the elastic constants, the vacancy formation energy, cohesive energy, and the lattice parameter of α-iron, and has been widely applied to various simulation studies on α-iron[2]. The specimen has a dimension of 10×10×10 in units of lattice parameter (a) with no periodic boundary conditions and with the (001) plane perpendicular to the z-axis as well as the [100] direction parallel to the x-axis. Both the uppermost and the lowermost atomic planes of the specimen were oppositely stretched along the z-axis with a speed of $5\times10^{-4}a/\tau$, where τ is 0.4ps. Before stretching, each specimen was preannealed at a temperature (10K or 300K), which was kept constant throughout the simulation run. The Newton's equations of motion of atoms were solved with using the Verlet's algorithm[3] and the temperature was controlled by Woodcock's method[4].

Three kinds of movie systems are applied to the visualization of the calculated numerical data generated by the present molecular-dynamics simulations. Each of the primitive pictures in the movies were made using the three dimensional graphics software AVS on SGI video system (enclosed in the broken line in Fig. 2). One of the movies is a "video movie", and the others are MPEG1 and VRLM animation's which are to be treated on an intercommunication network system such as the Internet. The "video movie" demonstrates the

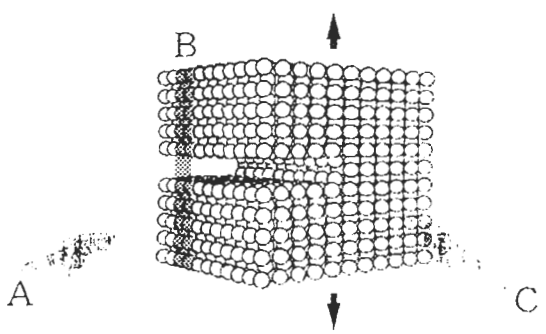

Fig. 1 Initial configuration of the present system. Details are written in the text.

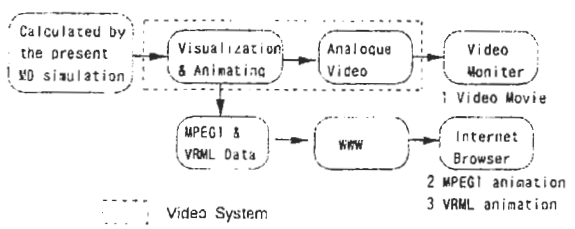

Fig. 2 Flow of the visualization of the calculated numerical data.

dynamical movement of atoms in both the whole crystal and a specific zone containing three adjacent atomic planes (indicated by the letter B in Fig. 1) in the crystal. One can make a discussion with his remote coworkers on the performance of pictures or the details of the studies using the MPEG1 animation system. Also one can rotate the pictures or look into the pictures from various view points by the VRLM animation system.

3. Results and Discussion

The deformation processes of the a-iron both at low temperatures and at high temperatures are shown in Fig. 3 and Fig. 4, where dark spheres indicate the atoms that were initially not in the specific zone but coming from the part other than the zone, and the other dark spheres indicate atoms having no nearest neighbors along the direction of the z-axis within the distance of 1.33a, which value is the truncation distance of the interatomic potential used in the present calculation. The crystal stretched at 10K is shown to be broken via cleavage mechanism accompanied by the cleavage surface parallel to the (001) plane (see Fig. 3). On the contrary, the crystal stretched at 300K is shown to be deformed and broken via slip mechanism initiated by dislocation emission at the crack tip (see Fig. 4). The slip system in this case has a {110} slip plane and <111> slip direction, which coincides with one of the slip systems observed in the tensile tests of the real α-iron crystals. The present results that the α-iron is brittle at lower temperatures and ductile at higher temperatures are indeed the case for the real α-iron crystals.

In addition to the above, an icosahedron with twenty faces is observed to form very shortly before the overall fracture in the vicinity of the neck of the deformed crystal stretched at 300K (see Fig. 5). Once the icosahedral structure was formed, despite of being under the constrained state, the icosahedron was observed to be rather stable throughout the simulation run. In connection to this, it may be pronounced that the deformation mechanism of the neck region formed at the very last stage of the present simulation is not of the usual slip mechanism but of some other mechanism that has not been characterized yet. According to the fact that the present results fully reproduce the actual fracture properties of the real α-iron crystals, it may be predicted that some icosahedral structure should be also formed at the last stage of the fracture of the real α-iron crystals.

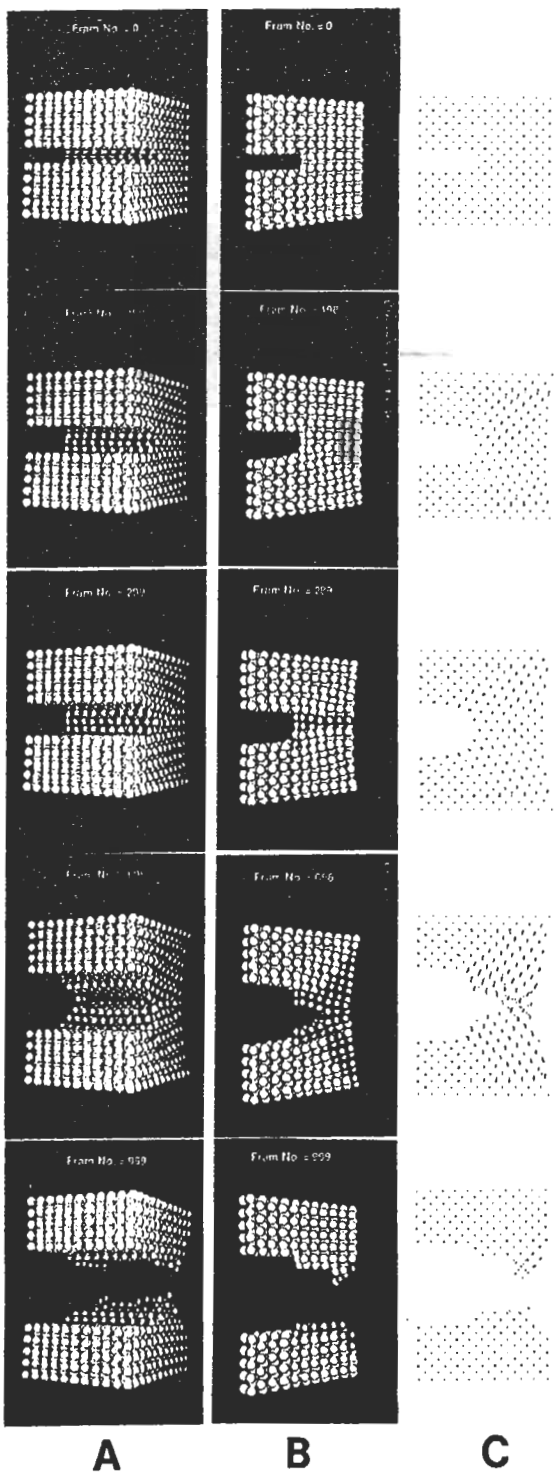

Fig. 3 Mode-I fracture process of α-iron crystal at 10K. Details are discussed in the text.

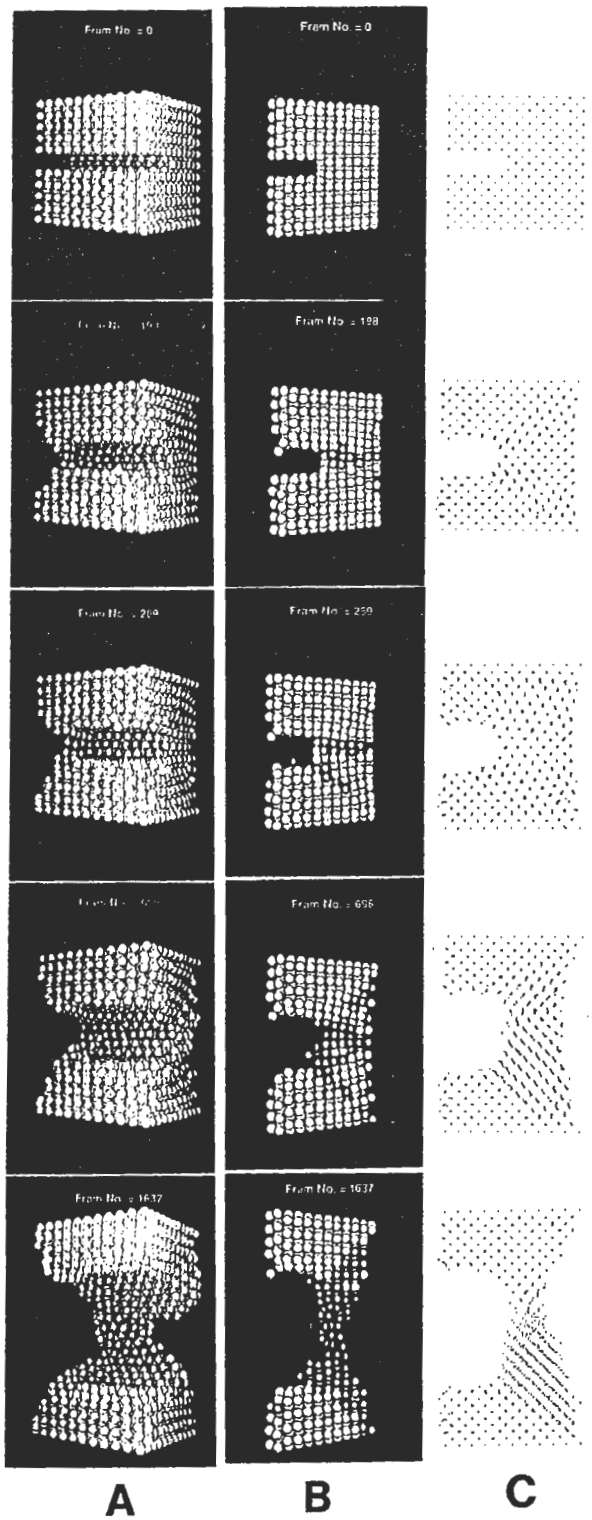

Fig. 4 Mode-I fracture process of α-iron crystal at 300K. Details are discussed in the text.

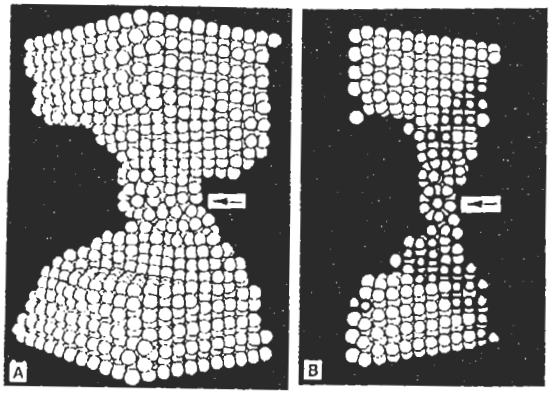

Fig. 5 An icosahedron (indicated by an arrow) appearing at the last stage of the Mode-I fracture process of the α-iron crystal at 300K. Details are discussed in the text.

4. Conclusion

Atomistic processes of the mode-I fracture of α-iron constructed with the Johnson's interatomic potential are simulated by molecular-dynamics calculations and the resultant huge amount of numerical data are demonstrated by movies. In case when the α-iron crystals with an initially introduced crack are stretched along the [001] direction, it is shown that the bcc-Fe is intrinsically brittle at lower temperatures and ductile at higher temperatures. The fracture of α-iron at lower temperatures is shown to take place by propagation of a crack along a (001) plane of the iron crystals. On the contrary, the fracture of the crystals at higher temperatures is shown to occur by plastic deformation initiated at around the initially introduced crack tip. These results are consistent with the case of the tensile behavior of the real α-iron crystals. An icosahedron with rather stable structure is observed to form at the neck of the specimen shortly before an overall rupture in the high temperature deformation process.

References

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