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# Computer simulation of vacancy migration in copper

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A migration of a single vacancy and a di-vacancy in copper at high temperature is studied by the molecular dynamics simulation with the EAM potential. The crystal which is utilized in the present work consists of 4000 atoms (the size = $10a_0$x$10a_0$x$10a_0$ where $a_0$ is the lattice constant). Simulations of single vacancy migration were carried out at five temperature (950K, 1000K, 1100K, 1200K, 1300K) and that of di-vacancy were carried out at four temperature (650K, 700K 750K, 800K). The migration energy of single vacancy and di-vacancy, which was calculated from temperature-dependent of jump interval, was 0.71 eV and 0.22 eV respectively. Successive jumps of a single vacancy which occurs at very short interval were observed at 1200K and 1300K. In case of a single vacancy migration, an atom have to pass saddle point gate which four atoms of the nearest neighbor form. When an atom trying to jump is on saddle-point, the gate expands. After an atom passes saddle-point, the gate shrinks. Because the gate shrinks, the nearest gate expands and the subsequent jump occurs easily. The vibrational frequency of atoms of the nearest neighbor of a vacancy was examined by Fourier-transform of the time-dependent displacement. The vibrational frequency to a vacancy is lower than that of atoms in normal site.

## 1 Introduction

The activation energy for migration of vacancies in copper have been investigated experimentally by measurement electric resistivity of quenched and irradiated samples [1]. There are many experimental results. Also migration energy was calculated from energy of saddle point configuration on diffusion path [2]. In the present work the migration energy of single and di- vacancy was investigated by carrying out molecular dynamics computer simulation at high temperature.

## 2 Procedure

Computer simulations of molecular dynamics were carried out with the code DYNAMO that developed by Daw, Foiles and Baskes in Sandia National Laboratory in Livermore. The EAM potential of copper that is utilized in the present simulation was parameterized by T. Diaz de la Rubia with the Foiles' procedures[3]. The crystal which is utilized in the present work consists of 4000 atoms ($10a_0$x$10a_0$x$10a_0$ where $a_0$ is the lattice constant). Simulations of single vacancy were carried out at five temperature (950K, 1000K, 1100K, 1200K, 1300K) and that of di-vacancy were carried out at four temperature (650K, 700K 750K, 800K). The migration energy of single vacancy and di-vacancy was calculated from temperature-dependent of jump interval. The frequency of atoms which was the first-nearest neighbor of a vacancy was examined by Fourier-transform.

Table 1 the migration energy of single vacancy and di-vacancy

| | | migration energy | 0 |
|---|---|---|---|
| single vacancy | present work | 0.71 | |
| | saddle point energy | 0.63 | |
| | quench | 0.77 | Lucasson et al.(1964) |
| | quench | 0.85 | Wright and Evans(1966) |
| | quench | 0.74 | Schilling et al.(1970) |
| | irradiation | 0.67 | Meechan et al.(1960) |
| | irradiation | 0.71 | Dworschak and Koehler(1965) |
| | irradiation | 0.69 | Brugiere and Lucasson(1968) |
| | irradiation | 0.72 | Schilling et al.(1970) |
| | irradiation | 0.7 | Wienhold et al.(1978) |
| di-vacancy | present work | 0.22 | |
| | saddle point energy | 0.33 | |
| | quench | below 0.68 | H. W. Schamp and Thesis |

## 3 Result

Table 1. shows the migration energy of single vacancy and di-vacancy which was calculated in the present work, calculated from saddle point configuration of diffusion path and experimental result. The migration energy of single vacancy was good agreement with experimental results. The migration energy of di-vacancy was lower than experimental results. But there are only a few experimental results and the value aren't determined correctly, because obtaining the migration energy of di-vacancy was very difficult. Comparing with saddle point energy of di-vacancy, the value seems to be in reasonable range.

Successive jumps of a single vacancy which occurs at very short interval were observed at 1200K and 1300K. For single vacancy diffusion, an atom have to pass a rectangular gate which four neighbor atoms on same (110) plane form. Fig. 1 shows the sum of diagonal length of a gate versus elapsed time; the arrow indicates the time when one jump occurs. When an atom trying to jump is on saddle-point, the sum is higher than that of perfect crystal. It means the gate expands. After an atom passes saddle-point, the sum is lower than that of perfect crystal. It means the gate shrinks. Configuration of atoms trying to jump and forming two gates is shown in fig. 2. This is an example of successive jumps of a single vacancy which occurs at very short interval. When the first jump finish, the first gate shrinks. And the shape of the second gate changes, for these two gates contain one atom jointly.; big circle indicates an atom contained jointly. Because of displacement of an atom contained jointly, the second jump occurs easily.

When single vacancy diffuses, an atom trying to jump passes center of the gate. But in case of di-vacancy, it is shown in fig. 3, an atom trying to jump doesn't passes center of the gate and passes place close to vacancy of the gate.

Fig. 4 shows the displacement of an atom of the nearest neighbor of a vacancy versus the elapsed time and the Fourier spectrum of the time-dependent displacement. The obtained vibrational frequency is $1.4 \times 10^{12}$ and $1.2 \times 10^{12}$ for single vacancy and di-vacancy respectively.

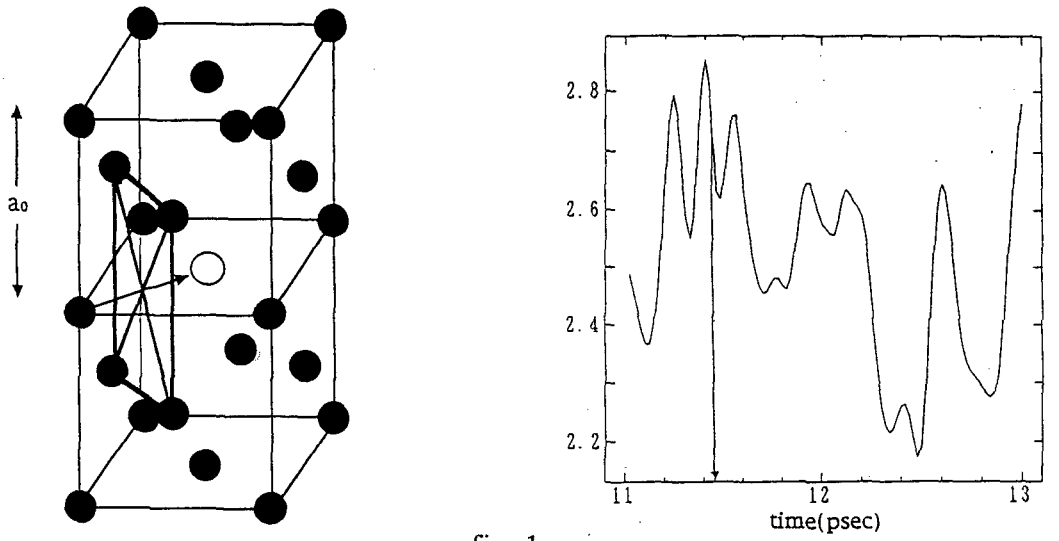


fig. 1

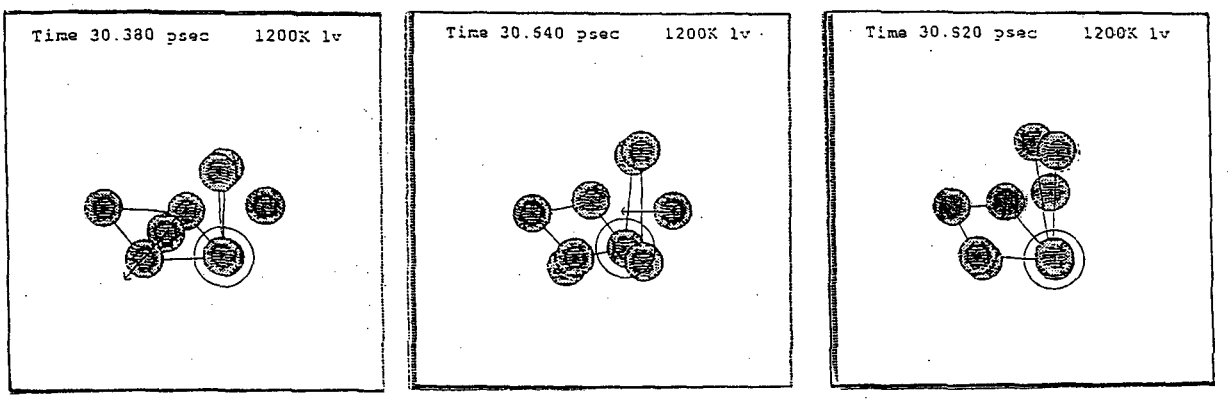


fig. 2

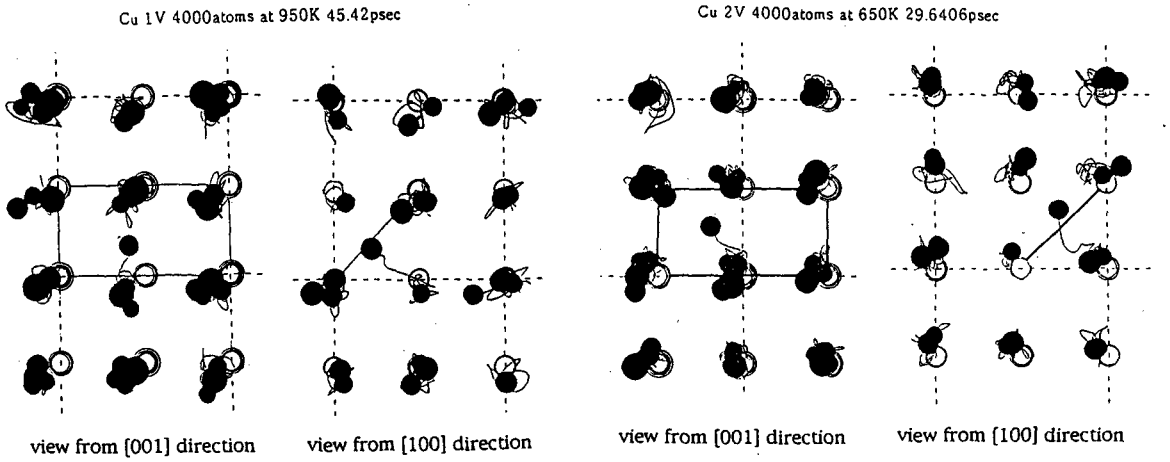


fig. 3

## 4 Conclusion

1. The migration energy of single and di- vacancy is 0.71 eV and 0.22 eV respectively.
2. Successive jumps of a single vacancy which at very short interval were observed at 1200K and 1300K. When vacancy migration , the saddle point gate, which four neighbor atoms on same (110) plane form, expand and shrink. And subsequential jump occurs easily.
3. An atom trying to jump doesn't pass center of the gate. It passes place close to vacancy of the gate.
4. The vibrational frequency is $1.4 \times 10^{12}$ and $1.2 \times 10^{12}$ for single vacancy and di-vacancy respectively.

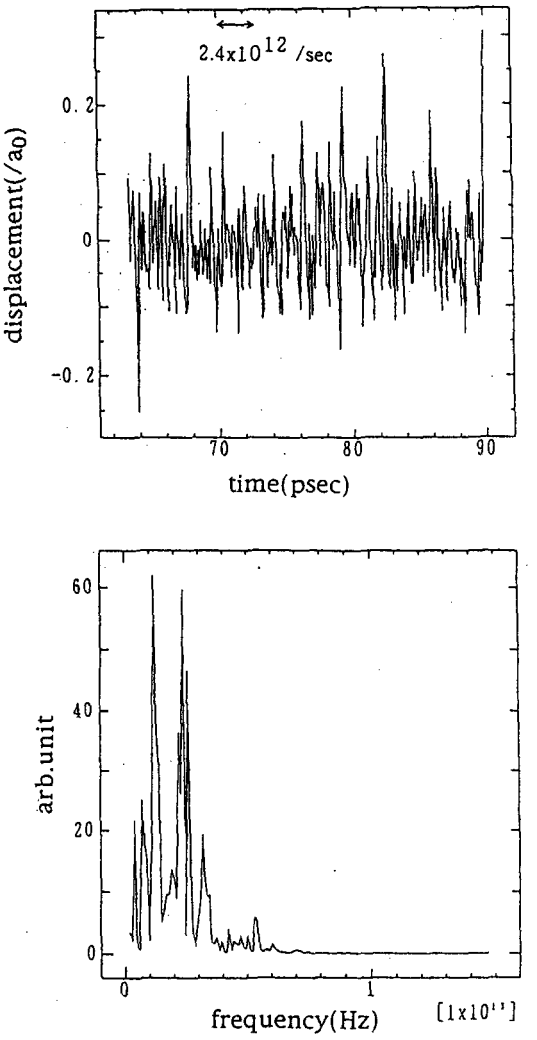


fig. 4

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2. Y. Shimomura, R. Nishiguchi, T. D. de la Rubia and M. W. Guinan, "Proceedings of the Fourth International Symposium on Advanced Nuclear Energy Reserch", p. 372.
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