A COMPUTER SIMULATION OF HIGH-DOSE ION IMPLANTATION INTO AMORPHOUS MATERIALS

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ABSTRACT

A computer program MACA was developed for simulating high-dose ion implantation into amorphous solids. The topology of amorphous solids was modelled by adjusting the free flight path distribution between collisions, so that the radial distribution function will characterize the short-range order and long-range disorder of amorphous targets. A simulation example is given.

Key words: Simulation of high-dose ion implantation Amorphous target topology modelling MACA code

With ever increasing requirements of microelectronic device fabrication, multiple high-dose ion implantation has become more attractive in recent years. For studying the effects of high-dose implantation and obtaining the desired parameters for experiments, a computer program MACA used on microcomputers has been developed. The characteristics of high-dose implantation are: dramatic change of target composition, amorphous phase formation and thermal effects caused by dose-rate. For this purpose, we have made somewhat detailed investigation of the topology of amorphous targets. So far as we have known, most commonly used methods of modelling amorphous targets use

$$f(r) = (1/a)\exp(-r/a) \tag{1}$$

as the distribution function of bond lengths (i.e. distances of coordination atoms), where a is average value of these bond lengths. This distribution of target atoms are totally random. However, the salient feature of a real amorphous solid is its short-range order and long-range disorder. Unfortunately, function (1) cannot reflect this nature. In this paper, a new distribution function

$$f(r) = [1/\sigma\sqrt{2\pi}]\exp[-(r-a)^2/2\sigma^2] \tag{2}$$

with $\sigma = 0.05a$ is assumed. With this normal distribution function, a planer network of atoms can be grown up from a convex quadrilateral seed by using certain computational method with random numbers. The random network so formed with the desired normal distribution of bond lengths is shown in Fig.1. Its RDF (Radial distribution function) as shown in Fig.2 demonstrates the similar nature of amorphous solid as determined by the method of EXAFS[1]. For comparison, the RDF of a square lattice network and that of gas calculated by the same method are shown in Fig.3. The

MACA code based on this model takes into account of target composition evolution during collision cascades without considering the thermal effects. Volume relaxation with atomic sizes of different elements is also considered. ZBL electronic stopping powers[2] are used in the program. Fig.4 shows an example as calculated by MACA. We obtain a uniform distribution of implanted N^+ ions in Fe target with concentration of about $5.5\times 10^{20}/cm^3$ up to about 400 nm. The doses corresponding to different energies of N^+ ions implanted are given as follows:

Energy (keV)	20	50	90	150	250	400
Dose(10^{15} ions/cm^2)	1.1	1.5	2.1	4.0	5.7	10.0

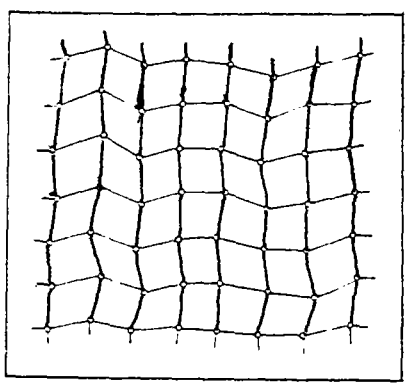

Fig.1 Sample random network determined by function(2)

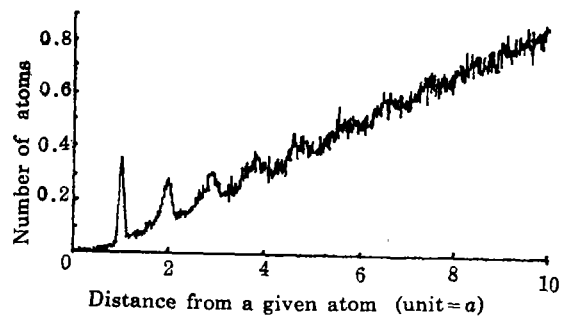

Fig.2 RDF of the sample random network

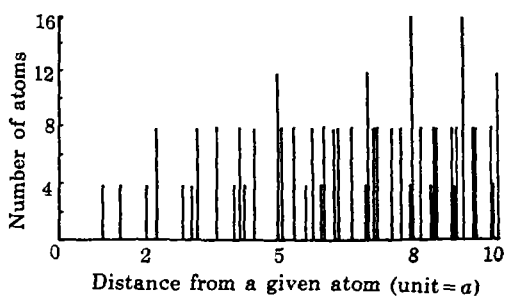

Fig.3 RDF of square lattice and gas

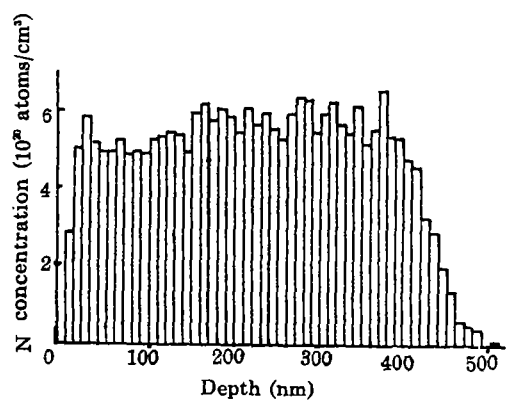

Fig.4 A desired distribution of N^+ implanted into Fe

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