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Comparative study of silicon and germanium sputtering by 1–20 keV Ar ions

V.I. Shulga *

Institute of Nuclear Physics, Moscow State University, 119992 Moscow, Russia

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Abstract

Sputtering of amorphous Si and Ge targets by 1–20 keV Ar ions has been studied using the binary-collision simulation. Special attention was given to the angular distribution of sputtered atoms; namely, the energy dependence of the exponent n in the function $\cos^n\theta$ approximating the angular distribution (θ is the polar ejection angle). It has been shown that at all incident energies the value of n for Ge is much higher than that for Si, which is in contrast with analytical predictions. The reasons for this discrepancy are discussed in detail. In addition, the simulated values of the sputtering yield are also considered and compared with the data from the literature.

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Keywords: Sputtering; Angular distribution; Sputtering yield; Silicon; Germanium; Computer simulation

1. Introduction

Silicon and germanium are of special importance in sputtering investigations. Both materials become amorphous at low ion bombarding fluences, which allows for an accurate comparison between experimental results and theoretical predictions usually made for structureless targets. Noteworthy also is the fact that silicon and germanium (and their composites) are very important materials in micro- and nanoelectronics. Plasma and ion beam technologies, which are extensively used in sputter-deposition systems, are examples of technologies that use these materials. The development of such technologies requires detailed information on all the characteristics of the sputtering process.

This paper addresses mainly the angular distributions of sputtered Si and Ge atoms. The interest in this study was motivated by the results of recent experiments [1,2] on sputtering of Si and Ge targets by 3–10 keV Ar ions at normal incidence. In these experiments, the Rutherford backscattering (RBS) technique was used to analyze the collected material. In both cases (Si, Ge) the target surface was found to be practically flat even at total fluence $\sim 10^{18}$ ions/cm^2 [2]. The angular spectra were approximated by the function $\cos^n\theta$ and the best-fit values of n were found. It turned out, that the angular distributions of sputtered atoms are overcosine and that $n \approx 1.3$ and 1.7 for Si and Ge, respectively. This is in contrast with a purely cosine ($n = 1$) angular distribution, which follows from the model of isotropic collision cascades, e.g. [3,4].

Fig. 1 presents all the experimentally reported data of n for Si and Ge targets under Ar ion bombardment [1,2,5–7]. Also shown are the theoretical predictions for keV- [8] and sub-keV ion bombardment [9]. Sigmund [8] took into account a net deflection of ejected atoms to the surface normal in the last (non-compensated) collisions and derived

$$n = 1 + (8/3)NC_0^{3/2}, \tag{1}$$

where N is the target atomic density and C_0 is the constant defined in [4]. Stepanova and Dew [9] suggested an

* Tel.: +7 495 939 3562; fax: +7 495 939 0896.
E-mail address: shulga@hep.sinp.msu.ru

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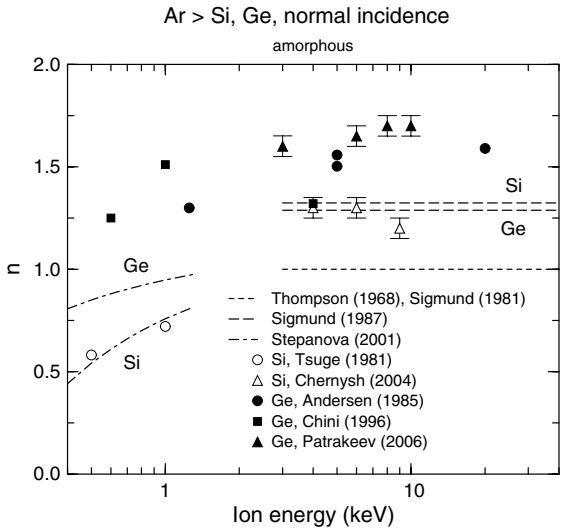

Fig. 1. Survey of predicted (lines) and measured (dots) values of n for amorphous Si and Ge targets sputtered by Ar ions at normal incidence. Lines: predictions made in [3,4,8,9]. Dots: experimental data from [1,2,5–7].

approximate semi-empirical description for the angular spectrum of sputtered atoms which takes into account not only the surface scattering (focusing) effect but also the anisotropy of collision cascades in terms of the theory by Roosendaal and Sanders [10].

From Fig. 1, it is obvious that Eq. (1) cannot explain the high experimental values of n for Ge in the energy range $E \gtrsim 5$ keV where the estimate [8] should work well. An attempt to understand this contradiction by the use of computer simulation technique is the aim of the present work. In addition, the simulated values of the sputtering yield will be also considered and compared with the data from literature.

2. Simulation

The simulations were performed using the computer code OKSANA [11]. The code is based on the binary collision approximation and takes into account weak simultaneous collisions at large distances. An amorphous target is simulated by rotation of a crystalline atomic block, the procedure of rotation being repeated from collision to collision. The atomic block is chosen in the form of a tetrahedron, which is the typical structure for crystalline Si and Ge. The model used was carefully tested in [12] by comparison of the simulated depth profiles of sputtered atoms with the results of the Monte Carlo program TRIM.SP, which assumes a random target. The standard WHB (KrC), ZBL and LJ potentials are applied as the interaction potential $V(R)$ for colliding particles, e.g. [13]. The inelastic energy losses were calculated by the Firsov formula. Allowance was made for the uncorrelated thermal vibration in terms of the Debye model ($T = 300$ K). The surface barrier is planar and the heat of sublimation (4.70 and 3.88 eV for Si and Ge respectively) is taken as the surface binding energy. The target atomic density N is 0.0498 and 0.0443 atoms/Å^3 for Si and Ge respectively. A flat surface at $x = 0$ is assumed. A typical run consisted of 200,000–500,000 sputtered atoms. All other parameters were identical with the standard model [14]. The simulated angular distributions of sputtered atoms, $Y(\theta)$, were fitted by the function $\cos^n\theta$ and the corresponding best-fit values of n were found.

For better understanding of the difference between the results for Si and Ge targets, some additional simulations of sputtering were carried out for several artificial pseudo-Si targets and for the model, in which the scattering of incident ions in the target was switched off (see subsequently).

3. Results and discussion

Fig. 2 compares the measured values of n with the results of computer simulations performed using different interatomic potentials. It is seen that for Ge the simulated values of n are quite sensitive to the variation of the potential. The ZBL potential provides the highest values of n while the WHB and LJ potentials lead to much lower values of n. The latter can be explained by a weakness of the WHB and LJ potentials for Ge at large distances which determine the scattering of particles during their ejection from the surface (see Fig. 6 from [15]). It is also seen from Fig. 2 that $n_{\mathrm{WHB}} > n_{\mathrm{ZBL}}$ for Si but $n_{\mathrm{WHB}} < n_{\mathrm{ZBL}}$ for Ge. Again, such a reverse of the WHB and ZBL data correlates well with the behavior of the relevant potentials [15]. The decrease of n at low ion energies (Fig. 2) can be explained by a high contribution of the primary knock-on atoms

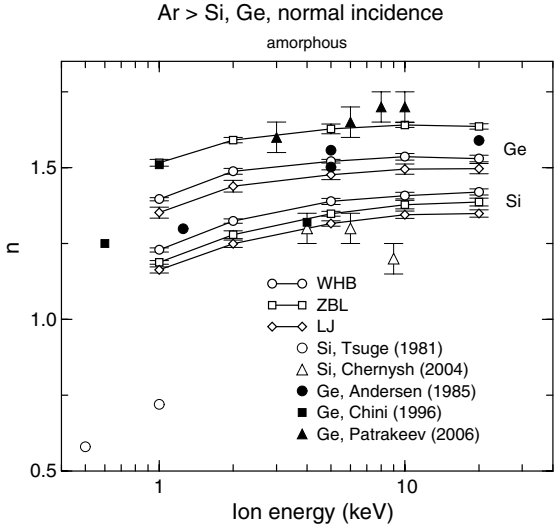

Fig. 2. The energy dependences of the exponent n for amorphous Si and Ge targets sputtered by Ar ions at normal incidence. Solid lines are the results of computer simulations performed using different (WHB, ZBL, LJ) interatomic potentials; dots are the experimental data [1,2,5–7].