Thermalization of sputtered atoms

Kevin Meyer,[a] Ivan K. Schuller, and Charles M. Falco
Solid State Science Division, Argonne National Laboratory, Argonne, Illinois 60439

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We have calculated the energy distributions of sputtered Nb and Cu atoms ejected from amorphous targets under low-energy Ar bombardment. A formula based on elementary kinetic gas theory is used to calculate the subsequent energy loss of the ejected atoms due to collisions in the sputtering gas. The energy distributions of the sputtered atoms arriving at the substrate is compared with the distributions obtained using thermal evaporation techniques. This comparison indicates that the preparation of epitaxial metallic films, such as Layered Ultrathin Coherent Structures using sputtering techniques may have fundamental advantages over thermal evaporation.

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I. INTRODUCTION

The engineering of novel materials using modern thin film techniques has received considerable attention recently. Semiconducting superlattices showing a high degree of epitaxy have been prepared using thermal evaporation techniques.[1] On the other hand, metallic layered ultrathin coherent structures (LUCS) have to date only been successfully prepared using sputtering techniques.[2,3] It is the purpose of this work to compare the energy distribution of particles arriving at the substrate for sputtering and thermal evaporation. It is expected that differences in these energy distributions might be responsible for variations in layered metals prepared by the two methods.

Several theories have been developed to describe the energy distribution of atoms sputtered from a target.[4] Although these theories differ in detail, as far as our calculation is concerned, these differences have only a minor effect on the end result. Thompson[5] has developed a theoretical model in which ejection results principally from the generation of collision cascades by the bombarding ion. We use this model to first calculate the initial energy distributions of sputtered Nb and Cu atoms from amorphous targets under low-energy ($\leqslant$410 eV) Ar bombardment. The subsequent thermalizing effect of the sputtering gas on particular energies in the distributions of sputtered Nb, Ge, and Al has been previously studied by Cadieu and Chencinski.[6] This treatment is extended here to include the thermalizing effect on the entire energy distribution, which ultimately determines the energy distribution of atoms arriving at the substrate.

In Sec. II we describe Thompson's model of the sputtering process, as well as discuss the formula used by Cadieu and Chencinski to determine the energy loss of the sputtered atoms due to collisions with atoms in the sputtering gas. Section III describes the calculation we have done to determine energy distributions, including the effect of interaction with the sputtering gas. Section IV contains the results of the present work.

[a]Participant in the 1980 Summer Energy Institute, June 11–August 15, 1980. This program is coordinated by the Argonne Center for Educational Affairs.

II. MODEL

The calculation is performed by using the Thompson model to obtain the initial energy distribution of particles ejected from a sputtering target. Subsequently, the sputtered particles are allowed to collide with the Ar sputtering gas, which is assumed to have a Maxwell-Boltzman distribution. The number of collisions, and hence the energy loss, is determined by the Ar pressure as well as target-substrate distance.

Thompson[5] has found that it is possible to quantitatively explain the initial energy distribution of sputtered ions as they leave the target by assuming that sputtering occurs due to the generation of atomic collision cascades caused by the bombarding ion. Assuming ejection results from both random collisions as well as focused collision sequences, the theory can account for 90% of the sputtering. The flux of sputtered atoms in this model is given by

$$\Phi(E,\varphi) d\Omega\, dE = P \cos\phi \frac{1 - [(E_b + E)/\Lambda E_1]^{1/2}}{E^2(1 + E_b/E)^3} d\Omega\, dE, \tag{1}$$

with

$$P = \frac{\pi a^2 \Lambda E_a \eta D \Phi_1}{16}, \qquad \Lambda = \frac{4M_1M_2}{(M_1 + M_2)^2},$$

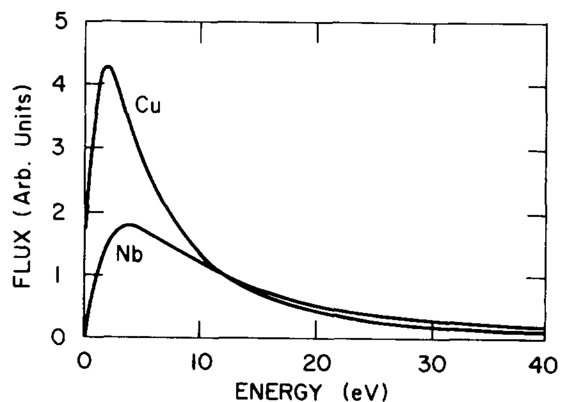

FIG. 1. Initial energy distributions for sputtered Cu and Nb at the surface of the targets. Argon gas accelerating voltage 410-V for Cu and 270 V for Nb.

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TABLE I. Parameters used in calculation of energy distributions.

	Nb	Cu
atomic mass M_2	92.9 g/mole	63.5 g/mole
atomic number Z_2	41	29
binding energy E_b	7.48 eV	3.49 eV
melting point	2741 °K	1356 °K
interatomic distance D	2.62 Å	2.28 Å
geom. cross section σ	27.9×10^{-20} m^2	24.9×10^{-20} m^2
target voltage	270 V	410 V
target power	1.34 kW	0.63 kW
gas parameters: Ar		
$T_G = 550$ °K	pressure = 10 mT	
$Z_1 = 18$	$E_g \leqslant 0.4$ eV	
$M_1 = 39.9$ g/mole		

and

$$E_a = \frac{2E_R(Z_1Z_2)^{7/6}(M_1+M_2)}{eM_2},$$

where ϕ is the ejection angle, E_1 is the energy of the incident ion, M_1 and M_2 are the respective masses of the ion and target atoms, ΛE_1 is the maximum recoil energy, $a = a_0/(Z_1Z_2)^{1/6}$ is the screening radius of the interatomic potential ($a_0 = 0.53$ Å), E_a is the value of E_1 that gives the distance of closest approach in a head-on collision, $\eta = 0.52$, D is the nearest-neighbor spacing in the target, E_R is the Rydberg energy, and Φ_1 is the flux of incident ions perpendicular to the surface of the target. The distribution given by Eq. (1) rises linearly to a peak near $\frac{1}{2}E_b$, falls initially like $1/E^2$, then becomes zero at ΛE_1. This behavior is in good agreement with experimental results (see for example, Stuart and Wehner[7]).

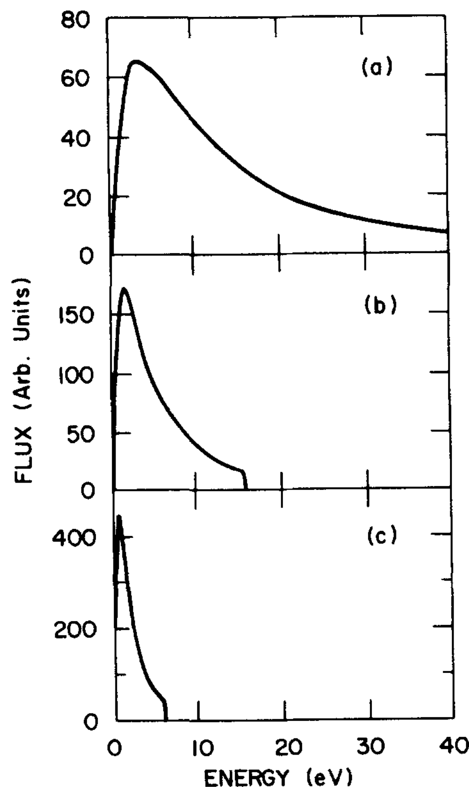

FIG. 2. Change in Nb energy distribution with distance from target with Ar gas pressure 10 mTorr. Distances are (a) 0 cm, (b) 3 cm, (c) 6 cm.

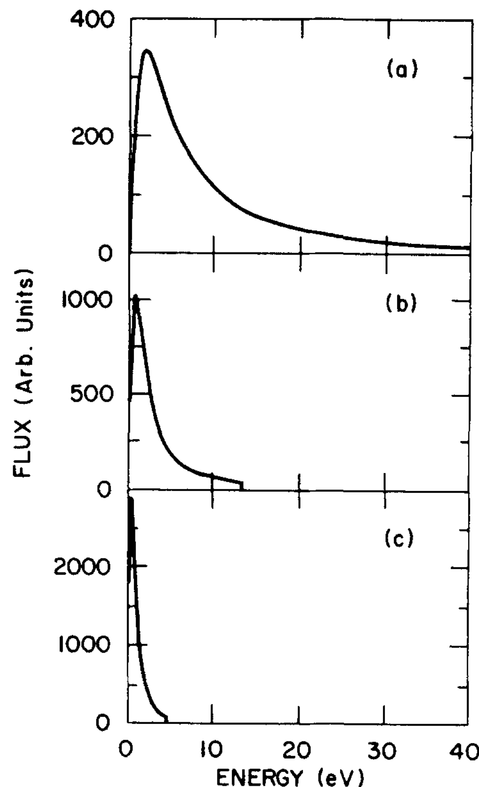

FIG. 3. Change in Cu energy distribution with distance from target with Ar gas pressure 10 mTorr. Distances are (a) 0 cm, (b) 3 cm, (c) 6 cm.

The energy loss of a sputtered atom as it passes through the Ar sputtering gas can be estimated from [4]

$$E_F = (E_0 - k_B T_G)\exp[n \ln(E_f/E_i)] + k_B T_G, \qquad (2)$$

where E_0 is the energy of the sputtered particle as it leaves the target, T_G is the sputtering gas temperature, E_f/E_i is the ratio of energies before and after a collision, and n is the number of collisions that take place in the gas. The number of collisions is given by

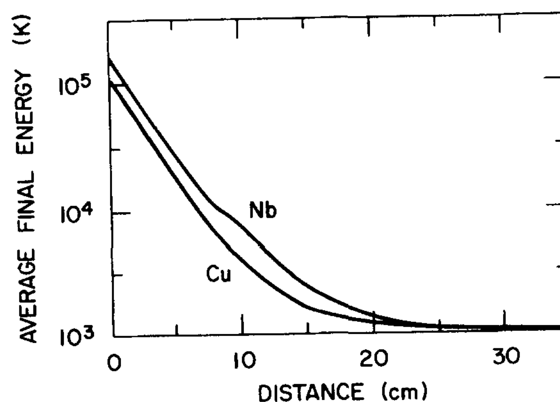

FIG. 4. Average Cu and Nb energies (expressed in units of temperature) as a function of distance from target. Ar gas pressure 10 mTorr and temperature 550 K. Note that this is the average energy, not the peak energy of the distribution.

$$n = dp\sigma/k_B T_G, \quad (3)$$

where d is the distance traveled, p is the sputtering gas pressure, and σ is the collision cross section assuming hard core interactions.

III. DETAILS OF THE CALCULATION

The energy distribution of the sputtered atoms at the surface of the target for a given set of sputtering conditions is calculated using Eq. (1). The subsequent evolution of this energy distribution as the atoms traverse the sputtering gas is then computed for various distances.

To calculate the energy loss of the sputtered atoms due to collisions with the sputtering gas, a Maxwell-Boltzman distribution at a temperature of 550 °K (typical in our experiments) has been assumed for the gas. Since we want to consider interactions with atoms of all of the possible energies in the gas (not just the peak energy), we replace $k_B T_G$ in Eq. (2) with E_g, a particular energy in the gas distribution. We then perform the energy-loss calculation for each energy E_g in the gas distribution to get a range of final energies for an energy E_0 of the sputtered atoms. This is repeated for each E_0 in the distribution of the sputtered atoms and weighted by the probability for that collision. This probability is simply the product of the value of the sputtering distribution $\Phi(E)$ and the value of the Maxwell-Boltzman distribution at E_g. These energy loss calculations are computed over all possible collision combinations. In this way we have arrived at the energy distribution of the sputtered atoms as they arrive at the substrate, for each particular gas pressure, target-to-substrate distance, and target voltage.

IV. RESULTS

Table I lists the input parameters used in our calculations. The operating parameters we have chosen (target voltages and powers, gas pressure, and temperature) are typical of those used in producing Nb/Cu LUCS thin films.[2,3]

Figure 1 shows initial energy distributions at the surface of targets calculated from Eq. (1) for sputtered Nb and Cu. The high-energy tails of the distributions extend to several hundred electron volts. However, for computational efficiency we have neglected atoms with energies higher than 40 eV since their numbers account for only a small percentage of the total population. In subsequent energy distribution curves a sharp cutoff is evident because we have disregarded these high energy atoms.

Figures 2 and 3 show how the shape of the sputtered atom's distribution changes with distance from the target. Eventually in the completely thermalized limit this distribution assumes that of the Ar gas distribution. Figure 4 indicates that with Ar used for the sputtering gas at a pressure of 10 mTorr, Cu atoms will thermalize after traveling a distance of about 20 cm from the target and Nb after about 25 cm. Since the energy distribution is Maxwell-Boltzman only in the thermalized limit, we have chosen to calculate the average energy for Fig. 4 rather than the peak energy. The peak energy does in fact occur at 550 K in this limit.

V. CONCLUSIONS

We have calculated the energy distribution of sputtered Cu and Nb atoms as a function of distance traveled through the Ar sputtering gas. Results have been presented for sputtering gas pressures, temperatures, and accelerating voltages which are typical of these conventionally used in preparing thin films. These results show that the energy of the sputtered atoms approaches the thermal energy of the sputtering gas within a few tens of centimeters. This calculation implies that sputtering offers some advantages over conventional thermal evaporation techniques for layered materials made of high melting point elements or compounds. The energy distribution of sputtered atoms arriving at the substrate is sharper than would be the case of evaporated atoms, deposited at the same rate. In addition, the energy of atoms arriving at the substrate can be adjusted to be substantially lower for sputtering than for thermal evaporation, with considerably reduced population in the high-energy tail of the distribution, so that the layered structure is damaged less by the atoms being deposited. By varying the sputtering conditions it is also possible to deposit atoms with effective temperatures equal to that of a heated substrate, thus promoting epitaxial growth in certain systems.

ACKNOWLEDGMENT

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