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PREFERENTIAL SPUTTERING OF BINARY COMPOUNDS: A MODEL STUDY

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A model classical dynamics calculation has been performed to ascertain the effect of atomic mass and surface binding energy on preferential sputtering in binary systems. We find the mass effect not to have a simple dependence on the ratio of the masses of the two components. Rather, for two binary systems, both with a mass ratio of ~3, the ejection yield of the lighter component can vary from being the same as that of the heavier component to being 100% larger. Over a limited range of surface binding energies the ejection yield is inversely proportional to the binding energy. In addition, we suggest that the effective scattering sizes should be considered as a possible cause for preferential sputtering.

1. Introduction

The ejection of particles from solids due to bombardment by energetic (500–5000 eV) ions is of importance in many experiments. The sputtering of particles may be a desired effect such as in secondary ion mass spectrometry (SIMS) where the nature of the ejected particles reveals something of the original configuration of the surface. On the other hand, sputtering of neutral particles from the walls of the chamber into the plasma in a tokamak causes an unwanted cooling effect. There has been considerable effort spent both experimentally and theoretically to gain a fundamental understanding of the ion bombardment process.

One aspect of the ion bombardment process which is difficult to isolate experimentally is preferential sputtering in binary compounds. One of the components can and often does eject at a faster rate than the other [1]. Several factors such as mass, binding energy, and/or vapor pressure differences between the components have been attributed to inducing preferential ejection [2–11]. To vary these parameters independently is virtually impossible experimentally. To simplify the problem, a number of studies have been initiated using particles from isotopically mixed compounds to focus solely on the mass

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effect. These studies show there is an enhancement in the ejection of the lighter component in the direction normal to the surface [12–14]. A simple scattering argument based on relative masses has been used to qualitatively explain this enhancement [14]. Observing this effect in systems with a larger ratio of masses is virtually impossible experimentally, since unless isotopes are used, the binding energy of the solid is also simultaneously changed. The task of finding a binary system in which the mass is constant and only the binding energy or vapor pressure is altered is considerably more difficult. Attempts to theoretically determine the causes of preferential sputtering have been pursued by several workers [2–11]. The majority of these theories are statistical in nature and presuppose a specific mechanism of ejection. For example, one such theory initially assumes that the ejection of particles is due entirely to direct interactions with the primary ion. In contrast to these statistical models, Kelly has performed a molecular dynamics calculation for a system of copper isotopes [11]. He was primarily concerned with differences in the angular distributions of the ejected isotopes.

In this study we describe the ion bombardment of binary compounds by a classical dynamics model. This model has been used extensively to reproduce, explain and predict many aspects of the sputtering process [15–20]. The advantage of this method is that the mass and binding energy can be independently varied over a wide range of values. In addition, the important ejection mechanisms can be determined from the calculations and do not have to be assumed in an a priori basis using one's intuition. It is beyond the scope of this method, however, to examine the effect of vapor pressure on the ejection yields.

To analyze the effect of mass on preferential sputtering our approach is to create hypothetical systems that have the masses of oxygen, copper and gold, but have a constant interaction potential or binding energy. Likewise, we may examine systems where the mass is fixed at 63.54 amu (copper) but the binding energy is varied over a wide range. In this work, we find that the mass effect does not correlate well with the mass ratio of the two components. For some systems with a mass ratio of the components as large as 4 there is no enhancement of the yield of the lighter component over that of the heavier component. Individual mechanisms can be found, however, which enhance either light or heavy particle ejection. Other models have predicted mass effects as large as a factor of 3 for the same mass ratio of the binary components [2]. Over limited ranges of binding energy we find that the yield is inversely proportional to the binding energy. Of course, the binding energy of each component must be appropriate for the compound and not for the pure substane. For large variations in binding energy the proportionality relationship breaks down entirely.

2. Description of the calculation

A classical dynamics approach is used to investigate the effect of mass and binding energy in the ejection process of binary compounds. Briefly, the solid is approximated by a microcrystallite of 4 layers with ~60 atoms per layer (fig. 1). The primary ion, Ar^+, in all cases reported here, bombards at normal incidence with 600 eV of kinetic energy. Hamilton's equations of motion are numerically integrated to determine the final positions and momenta of all the particles [15–20]. To allow for simultaneous interactions in the collision process we assume the interaction potential to be pairwise additive among the atoms in the system. For the Ar^+–substrate interaction the pair potential has the form

$$V = A\,e^{-BR}, \quad R \leqslant R_a, \tag{1a}$$

$$V = 0, \quad R > R_a, \tag{1b}$$

where R is the distance between the two atoms. These potential parameters are held constant for all the studies presented here and have the values, $A = 71.3$ keV, $B = 4.59$ Å^{-1}, and $R_a = 2.56$ Å. For the substrate–substrate interaction, the potential has the form

$$V = A\,e^{-BR}, \quad R \leqslant R_a, \tag{2a}$$

$$V = D_e \exp[-\beta(R - R_e)]\{\exp[-\beta(R - R_e)] - 2\}, \quad R_b \leqslant R \leqslant R_c, \tag{2b}$$

$$V = 0, \quad R \geqslant R_c. \tag{2c}$$

To connect the exponential repulsion at short range ($R \leqslant R_a$) to the Morse function at long range ($R \geqslant R_b$) a cubic spline is used [16]. The potential parameters for eq. (2) are given in table 1.

The basic substrate system considered here is a face centered cubic crystal of lattice constant 3.62 Å with the (001) face exposed. To ascertain the effect of mass on the ejection process three different masses are used: 16.0 amu, 63.54

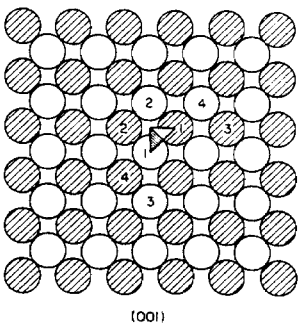

Fig. 1. Representation of (001) crystal face. The triangles are the impact zones for the single element and binary compounds. The numbers are labels used in the text.

Table 1
Potential parameters for the substrate–substrate interactions [a]

Potential	D_e (eV)	R_e (Å)	β (Å^{-1})	R_a (Å)	R_b (Å)	R_c (Å)
P1	0.18	2.628	1.405	1.90	2.44	4.34
P2 [b]	0.33	2.628	1.405	1.88	2.37	4.34
P3	0.48	2.628	1.405	1.50 [c]	1.99 [c]	4.34
P4 [d]	0.60	2.628	1.405	1.83	2.24	4.34
P5	0.73	2.628	1.405	1.81	2.17	4.34

[a] $A = 22.56$ keV, $B = 5.088$ Å^{-1} for all cases.
[b] The parameter D_e of P2 is an average of the D_e of P1 and P3.
[c] A slightly different procedure was used to determine R_a and R_b for $D_e = 0.48$ eV, so that there is not a continuous variation of the cutoff distances as a function of D_e.
[d] The parameter D_e of P4 is an average of the D_e of P3 and P5.

amu, and 197 amu (oxygen, copper, and gold, respectively). Crystallites of three types were examined. First, three calculations were performed in which all atoms in the crystallite have either the mass of oxygen, copper or gold, denoted by O/O, Cu/Cu and Au/Au, respectively, in table 2. Second, the atoms in the bottom three layers of the crystallite have the mass of copper while the atomic mass in the first layer is either that of oxygen (O/Cu) or gold (Au/Cu). In addition, four mass "alloy" systems were constructed. The top layer consists of an ordered arrangement of atoms of 2 different masses (fig. 1). The bottom three layers have the same mass. Their symbol in table 2 is of the form Cu–O/O which denotes that the first layer is composed of atoms with the masses of copper and oxygen while the mass of the atoms in the bottom three layers is that of oxygen. In all the alloy systems the shaded atoms in fig. 1 are the ones with the copper mass. For all the systems the potential P3 of table 1 is used.

Table 2
Systems for examining the mass dependence

Description [a]	Mass of particles in layer 1	Mass of particles in layers 2–4
Cu/Cu	63.54	63.54
O/O	16.00	16.00
Au/Au	197.00	197.00
O/Cu	16.00	63.54
Au/Cu	197.00	63.54
Cu–O/O	63.54, 16.00 [b]	16.00
Cu–O/Cu	63.54, 16.00 [b]	63.54
Cu–Au/Cu	63.54, 197.00 [b]	63.54
Cu–Au/Au	63.54, 197.00 [b]	197.00

[a] The potential in all cases is P3.
[b] For the "alloy" systems, the Cu mass is placed in the sites that are shaded in fig. 1.

To determine the effect of binding energy on the ejection process the mass of all the substrate atoms is held fixed at 63.54 amu (copper). A total of five different Morse potential well depths D_e are used. The potentials P1, P3 and P5 are used for three of the five systems. This results in binding energies for the solid of 1.80, 4.82, and 7.32 eV, respectively. These systems are denoted Cu^w, Cu/Cu, and Cu^s in table 3. Here the binding energy, E_b, has been defined to be the potential energy evaluated from eq. (2) for all neighboring atoms with a distance R_c of a surface atom in the undamaged crystallite. The other two systems are "alloy" systems where neighboring atoms have different binding energies. In each case the shaded atoms of fig. 1 and the atoms in the bottom 3 layers used P3 as their mutual pair interaction potential. The remaining (unshaded) first layer atoms have P1 (weak alloy–Cu^w_{alloy}) or P5 (strong alloy–Cu^s_{alloy}) as their mutual potential. The potential between the two types of atoms is either P2 or P4 for the weak or strong alloy, respectively. This array of systems allows a large variation of masses, 16–197 amu, and binding energies, 1.80–7.32 eV. From this independent variation of parameters, their influence on the ejection process can be studied in detail.

Although both the model mass and binding energy alloys only have two components in the first layer, we feel they are representative of binary compounds. As is discussed below, most of the particles which are ejected or sputtered during the ion bombardment process originate from the first layer. In addition, many of the collision processes which give rise to the sputtering involved primarily atoms in the first layer. Thus, although only the first layer of atoms contains two components we feel this is the most important region for the sputtering or ejection process.

For the system with only one type of mass or potential in the surface layer the zone of irreducible symmetry in which the Ar^+ ion bombards, is shown in fig. 1 by the small shaded triangle. For systems with two masses or potentials the impact zone is the larger right triangle. Experimental observables are

Table 3
Systems for examining the binding energy dependence

Description [a]	Binding energy of atoms in layer 1 (eV)	Potentials used
Cu^w	1.80	P1
Cu^w_{alloy} [b]	3.04	P1, P2, P3
	4.22	
Cu/Cu	4.82	P3
Cu^3_{alloy} [b]	5.28	P3, P4, P5
	6.24	
Cu^s	7.32	P5

[a] The mass of all the particles is 63.54 amu.
[b] See text for a description of these systems.

determined by averaging the results from the Ar^+ ion impacting at 50–100 evenly spaced points within the appropriate zone.

3. Results and discussion

The effect of mass and binding energy on the total ejection yield (number of particles ejected per incident ion) and on some specific ejection mechanisms will be discussed. The ejection yields for the various systems are given in tables 4 (mass effect) and 5 (binding energy effect).

3.1. Mass effect

Several workers have given theoretical treatments of the mass effect in preferential sputtering of binary compounds [2–11]. The arguments are generally statistical in nature and assume randomness of the processes. In addition, some workers assume that the incident primary ion's energy and/or direction of travel is not significantly altered after the first collision. Almost always an assumption of mechanism is made. The surface atoms are usually assumed to eject by either interaction with the primary ion or by collisions with upward moving atoms from below the first layer. The effect of the mass ratio on the sputtering depends strongly on the mechanism that is presupposed. The problem still remains to determine the relative importance of each mechanism. In addition, the validity of the assumptions must be ascertained.

The classical dynamics procedure allows one to determine the mechanisms of ejection and their relative importance. Of particular note is the observation that 30–50% of the ejection arises from collisions within only the first layer. As discussed below, many atoms eject due to the primary ion pushing the surface target atom down, which by conservation of momentum pushes up on its neighbor, forcing the latter particle to move or eject into the vacuum. Although this process involves first layer atoms, the second layer does influence the process. To our knowledge this has not previously been discussed as an important mechanism in preferential sputtering although other dynamics calculations have shown its importance [15]. Also of note is the fact that the energy and direction of the primary ion is significantly altered after the first collision.

In the studies of the mass alloy systems, Cu–O/O, Cu–O/Cu, Cu–Au/Cu and Cu–Au/Au, we only find appreciable enhancement of the yield of the lighter mass component in the Cu–O/O system and slight enhancement in the Cu–Au/Cu system (see table 4). The cause of this enhancement is that the heavy particle can easily backscatter the light particle but the reverse is not true [14]. In both the Cu–O and Cu–Au systems, the lighter mass substrate causes a larger preferential sputtering effect than the heavier substrate. Once the heavier particle gets a downward component of momentum, the lighter atom in layers 2–4 is virtually incapable of ejecting it.

Table 4
Numbers of particles ejected

	Cu/Cu	O/O	Au/Au	O/Cu	Au/Cu	Cu–O/O	Cu–O/Cu	Cu–Au/Cu	Cu–Au/Au
Number of impact points	211	66	66	66	66	119	119	119	119
Number of Ar^+ ejected	169 (0.80) [a]	1 (0.02)	66 (1.00)	53 (0.80)	42 (0.64)	12 (0.10)	93 (0.78)	91 (0.76)	116 (0.97)
Total number of Cu ejected	857 (4.06)	–	–	54 (0.82)	1 (0.02)	120 (1.01)	327 (2.75)	214 (1.80)	246 (2.07)
Number of Cu ejected from layers 2–4	4	–	–	54	1	–	73	5	–
Total number of O or Au ejected	–	213 (3.23)	183 (2.77)	250 (3.79)	193 (2.92)	223 (1.87)	318 (2.67)	172 (1.45)	241 (2.03)
Number of O or Au ejected from layers 2–4	–	2	4	–	–	5	–	–	26
Total yield of Cu and O or Au	4.06	3.23	2.77	4.61	2.94	2.88	5.42	3.24	4.09
Ratio of yields (light/heavy)	–	–	–			1.86	0.97 1.25 [b]	1.24	1.02 1.14 [b]
Ratio of masses (heavy/light)	–	–	–			3.97	3.98	3.10	3.10

[a] The numbers in parentheses are averages over the number of impact points.
[b] Ratio including only those atoms which eject from the first layer.

Table 5
Number of particles ejected

	Cu^w	Cu^w_{alloy}	Cu/Cu	Cu^s_{alloy}	Cu^s
Number of impact points	66	55	211	55	66
Number of Ar^+ ejected	52 (0.79) [a]	45 (0.82)	169 (0.80)	47 (0.86)	53 (0.80)
E_b (eV)	1.80	3.04	4.82	5.28	7.32
Number of particles ejected	417 (6.32)	159 (2.89)	857 (4.06)	108 (1.96)	177 (2.68)
E_b (eV)	–	4.22	–	6.24	–
Number of particles ejected	–	117 (2.13)	–	86 (1.56)	–
Total yield of Cu	6.32	5.02	4.06	3.53	2.68
Ratio of yields (weak/strong)	–	1.36	–	1.26	–
Ratio of E_b (strong/weak)	–	1.39	–	1.18	–

[a] The numbers in parentheses are averages over the number of impact points.

The cases examined here have large mass ratios, 3.97 and 3.10 for the Cu–O and Cu–Au systems, respectively, yet the enhancement of the ejection yields are between 0 and 25% except for the Cu–O/O system where the effects are compounded because the mass of O is also less than the mass of the Ar^+ ion (see below). Other workers have suggested that the enhancement of the yield could be as large as a factor of 3 for these mass combinations and specific mechanisms of ejection [2].

For all the systems studied 30–50% of the total yield is due to ejection of particles from mechanisms involving primarily first layer atoms. These mechanisms are not complex. For example, if one atom is pushed down the neighboring atom moves up and can possibly eject. As a result these mechanisms should be observed for the majority of surface structures since most surfaces have coplanar neighbors. The atoms of interest are the ones labeled 2–4 in fig. 1. The target atoms, designated as atom 1, are only observed to eject a significant number of times in the O/Cu, Cu–O/Cu, and Cu–Au/Au systems. Atom 2 ejects since the Ar^+ ion reflects from atom 1 and then moves under atom 2, forcing it up. Atoms 3 and 4 eject since atom 1 moves under them and pushes them up. The regions of the impact zone which give rise to the ejection of atoms 3 and 4, however, are different. The mechanisms for the ejection of atoms 2–4 are usually high energy, primarily involving collisions

among first layer atoms, and are found very frequently. Also, these atoms give rise to the high intensity in the angular distributions at a polar angle of $\sim 45°$ in the $\langle 100 \rangle$ azimuths [17,18].

It is conceivable that although the overall enhancement of relative total ejection yields is small, for one or more mechanisms the enhancement could be larger, as proposed by others. Table 6 gives the contribution of each of the above mechanisms to the total yield. Also given for the mass alloy systems is the ratio of light particle to heavy particle ejection for each mechanism. Most ratios are between 0.5 and 2.0, that is, the mass effect is only a factor of ~ 2

Table 6
Contribution to yield by specific mechanisms: mass effect

	Atom number [a]				Total yield
	1	2	3	4	
Cu/Cu	0.01 [b]	0.62	0.75	0.82	4.06
	–	15 [c]	18	20	
O/O	–	0.02	0.58	0.82	3.23
	–	1	18	25	
Au/Au	0.14	0.28	0.56	0.71	2.80
	5	10	20	25	
O/Cu	0.69	0.05	0.52	0.84	4.61
	15	1	11	18	
Au/Cu	0.07	0.77	0.50	0.59	2.94
	2	26	17	20	
Cu–O/O	0.01	0.12	0.50	0.68	2.88
	–	4	17	24	
	–	(∞)	(0.4)	(0.8)	(1.86)
Cu–O/Cu	0.60	0.30	0.68	0.91	5.42
	11	6	13	17	
	(0.7) [d]	(14.0)	(0.4)	(1.6)	(0.97)
Cu–Au/Cu	0.05	0.69	0.55	0.60	3.24
	2	21	17	19	
	(0.7)	(0.6)	(2.1)	(1.1)	(1.24)
Cu–Au/Au	0.47	0.50	0.62	0.77	4.09
	11	12	15	19	
	(1.6)	(0.9)	(2.0)	(1.0)	(1.02)

[a] The atoms are defined in fig. 1.
[b] The first entry is the contribution to the total yield by the particular atoms.
[c] The second entry is the percentage contribution of this atom to the total yield.
[d] The number in parentheses is the ratio of the yield of the light component to the yield of the heavy component.

for systems which have mass ratios of 3–4. In addition the mass effect can enhance either light or heavy particle ejection. The only large enhancement is the ejection of atom 2 from the Cu–O systems. This mechanism, however, contributes very little to the overall yield, so cannot be counted as significant.

The physical picture of mass effect in scattering also explains the fate of the Ar^+ ion. The light oxygen atoms are virtually incapable of backscattering the heavier Ar^+ ion so virtually all of the Ar^+ ions are implanted in the systems where oxygen masses occur in layers 2–4. For a substrate of the massive Au, virtually all Ar^+ ions eventually leave the solid although they may penetrate during the collisions process. For the Cu substrate systems, ~80% of the Ar^+ ions eventually leave. As seen in table 5, the substrate binding energy has very little effect on the fate of the Ar^+ ion. When some of the first layer atoms have the mass of oxygen (O/Cu and Cu–O/Cu), a large number of second layer particles eject. In contrast, for the systems with Cu or Au in the first layer, the calculations predict negligible ejection from the second layer. This observation is in agreement with the secondary ion mass spectrometry results of Niehus and Bauer who measured the W^+ ion intensity as a function of Ag adsorption coverage on W(110) [21]. When the Ag coverage reached one monolayer, the W^+ ion intensity and thus ejection from the second layer disappeared.

The mass effect in the angular distributions has been shown to enhance the light particle ejection in the direction normal to the surface, $\theta = 0°$ [11,14]. Fig. 2 shows the polar angular distributions for the Cu–O/Cu and Cu–O/O systems. In both cases the light particles eject more frequently at normal angles and less frequently at $\theta \sim 50$–$70°$. The ratio of light/heavy ejection is shown as a function of polar angle θ for both the Cu–O and Cu–Au systems in fig. 3. This effect is more pronounced when the substrate is the lighter species. For all

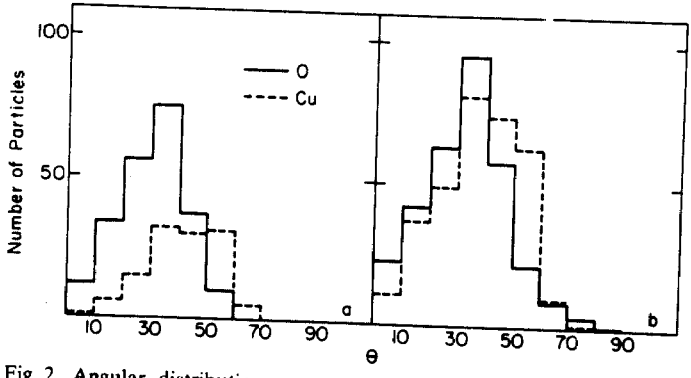

Fig. 2. Angular distributions versus polar angle, θ, measured from the surface normal; the histograms include atoms which eject at all azimuthal angles: (a) Cu–O/O, (b) Cu–O/Cu.

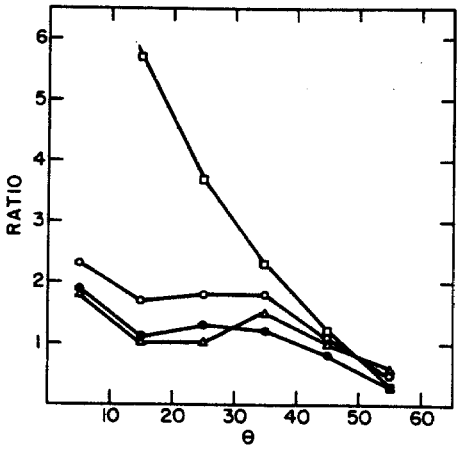

Fig. 3. Angular distributions: ratio of the yield of the light component to the yield of the heavy component. The points include atoms which eject at all azimuthal angles: (●) Cu–O/Cu, (□) Cu–O/O, (△) Cu–Au/Au, (○) Cu–Au/Cu.

the calculations we find virtually no particles ejecting with an angle of $\gtrsim 70°$. The azimuthal angular distributions of the O, Cu and Au are characteristic of a clean metal (001) face [17,18].

The total yields were plotted versus the hard sphere energy transfer ratio, γ, where

$$\gamma = \Delta E/E = 4m_1m_2/(m_1 + m_2)^2.$$

The quantities m_1 and m_2 are the masses of the Ar^+ ion and the substrate atom, respectively. This quantity is often included in statistical treatments to account for how much energy is effectively transferred to the system. The total yields do not increase monotonically with γ. The nonlinearity may lie in the fact that considerably more second layer ejection occurs when an atom with the mass of oxygen is in the first layer.

3.2. *Binding energy effect*

Experimentally measuring the influence of the binding energy of a substance on the sputtering yield is virtually impossible. However, it is thought to be a major contributor to the preferential sputtering effect. Most theories assume that the yield of particles that eject is inversely proportional to the binding energy of the atoms in the solid. In this work we examine a system where the binding energy is varied while holding the mass constant.

It is difficult to ascribe a unique binding energy to an atom in a solid. For the few particles that leave early in the collision cascade, the binding energy

could possibly be defined as the original static binding energy. The majority of the particles which eject, however, leave late in the collision process when there is considerable surface damage. Each ejecting particle experiences a different attractive force as it departs the solid. With this in mind, the following discussion refers to a binding energy (E_b) which is the potential energy of a surface particle in the original unperturbed lattice. This definition neglects relaxation of the crystal after one atom has been removed.

The results of the calculations for the copper mass system with varying binding energy are given in table 5. Plotted in fig. 4 are the yields versus $1/E_b$. For the single potential systems the calculated yields have been reduced by a factor of 2 so that they are comparable with the potential alloy systems on a yield per surface particle basis. Very few of the edge atoms eject so that the microcrystallite can be considered infinite with an equal mixture of components.

For small changes in the binding energy, the yield varies approximately linearly with $1/E_b$. This linearity breaks down, however, for larger changes in $1/E_b$. Calculations with slightly unphysical values of E_b (0.5 and 10 eV) were also performed to ascertain that the non-linearity was not due to statistical deviation. The curve is definitiely not linear over the entire region of $1/E_b$.

The ejection process requires that there be the proper sequence of collisions to give an atom an upward component of momentum. No matter how small the binding energy there must be a collision to initiate the ejection process. This point is illustrated in table 7. For example, atom 3 ejects in 64% of the Ar^+ ion impacts in the Cu^s case. This only increases to 86% in the Cu^w case

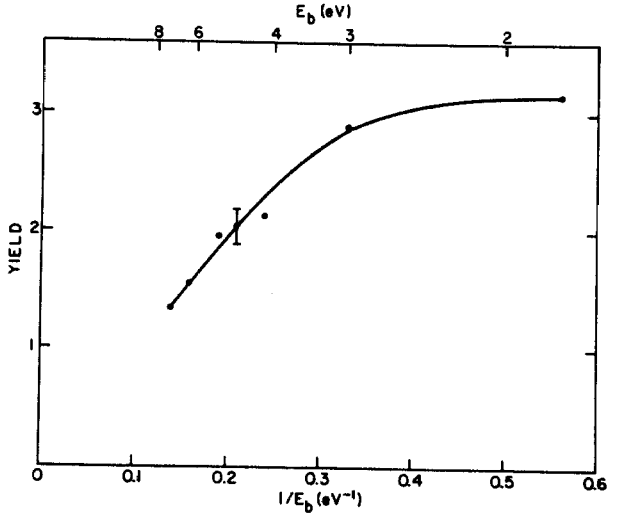

Fig. 4. Ejection yield versus binding energy, E_b.

Table 7
Contribution to yield by specific mechanisms: potential effect

	Atom number [a]				Total yield
	1	2	3	4	
Cu^w	0.20 [b]	0.82	0.86	1.03	6.32
	3 [c]	13	14	16	
Cu^w_{alloy}	0.05	0.66	0.75	0.98	5.02
	1	13	15	20	
	–	(1.0) [d]	(1.1)	(1.1)	(1.36)
Cu/Cu	0.01	0.62	0.75	0.82	4.06
	–	15	18	20	
Cu^s_{alloy}	–	0.58	0.62	0.83	3.53
	–	16	18	24	
	–	(0.9)	(1.1)	(1.3)	(1.26)
Cu^s	–	0.46	0.64	0.67	2.68
		17	24	25	

[a] The atoms are defined in fig. 1.
[b] The first entry is the contribution to the total yield by the particular atoms.
[c] The second entry is the percentage contribution of this atom to the total yield.
[d] The number in parentheses is the ratio of the yield of the weakly bound component to the yield of the strongly bound component.

where the binding energy is a factor of 4 times smaller. The mechanisms giving rise to the ejection of atoms 2–4 involve strong high energy collisions and are little affected by the binding energy. As the binding energy decreases more mechanisms may eject atoms but there are inherent saturation limits. Some regions of the impact zone of the incident ion will not give rise to the proper collision sequences to eject atoms. The percentages given in tables 6 and 7 reflect the choice of interaction potentials, primary ion energy and primary ion mass. Changing these values, however, should not alter the basic conclusions reached in either the mass or binding energy variation study.

In summary, although the yield of particles is inversely proportional to the binding energy over small changes in E_b, large extrapolations cannot be made. For alloy systems, the binding energy of importance is the E_b in the compound system and not of the pure substance. Interestingly, the binding energy has an effect on the angular distribution. The atoms with a smaller binding energy tend to eject more normally.

4. Summary

A classical dynamics calculation has been performed on model binary systems in order to examine the effect of mass and binding energy on

preferential sputtering. We find the mass effect not to have a simple dependence on the ratio of the masses of the two components. Rather, for two binary systems, both with a mass ratio of ~ 3, the ejection yield of the lighter component can vary from being the same as that of the heavier component to being 100% larger. We find that the light component tends to eject more in the direction normal to the surface, in agreement with experiment. This also agrees with recent conclusions by Kelly [2,22]. Although individual ejection mechanisms, e.g., direct interactions with the primary ion, may show large mass effects, the overall mass effect is relatively small.

The most important observation with respect to the analytic theories to come out of this calculation is that a new mechanism is found to play a dominant role in the ejection process. This mechanism involves primarily two collisions. First, the primary ion pushes one atom into the solid. This atom then exerts an upward thrust on its neighboring atom pushing this latter one into the vacuum. This process involves primarily atoms in the first layer. Although the actual frequency of occurence of this mechanism will depend on the components in the solid and the primary ion mass and energy, it should be an important factor in most real systems.

The binding energy, E_b, has a larger effect on the ejection yield than does the mass of particles. For a range of binding energies (~ 3–8 eV) the yield is inversely proportional to E_b. As E_b decreases, however, the yield saturates. No matter how small the binding energy, for an atom to eject there must be a collision sequence that gives the atom an outward component of momentum.

Besides the mass of the particles and the binding energy, structural factors, e.g., surface segregation [22], may cause the preferential ejection of one species. Another possible cause suggested by Watson and Haff [4b] but not generally discussed is the effect of the size of the atoms or scattering cross sections on the ejection probabilities. Although the size of the atoms is implicitly linked with the mass of a particle, these two effects are distinct. Examining the effect of size is outside the scope of this study but could be readily discerned by a classical dynamics procedure.

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