ON THE QUASI-THERMODYNAMICAL TREATMENT OF THE ENERGY DISTRIBUTION OF SPUTTERED PARTICLES

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Bombarding a crystal surface by an energetic ion beam in UHV causes sputtering. The emission of particles is due to the evolving collision cascades in the solids near to the surface. The energy distribution of the sputtered particles is given by the theory [1, 2, 3] as

$$f(E) = A \frac{E}{(E + E_b)^3} \tag{1}$$

where E_b is the surface binding energy and A is a constant.

The average energy of the emitted particles is given by:

$$E_{av} = \frac{\int\limits_0^{E_0} E \cdot f(E) \mathrm{d}E}{\int\limits_0^{E_0} f(E) \mathrm{d}E} \tag{2}$$

Using (1)

$$E_{av1} \cong E_b \left[2 \cdot \ln \left(1 + \frac{E_0}{E_b} \right) - 3 \right] \tag{3}$$

here E_0 denotes the highest energy possible of a sputtered particle and it is assumed that $E_0 \gg E_b$.

One of the authors has shown recently that (1) can be approximated in some energy region by a Maxwell type distribution [4]

$$F(E) = BE^{1/2} \cdot \exp \{- bE\} \tag{4}$$

where

$$b = E_b^{-1}$$

has to be used as fitting parameter and B is a constant.

The Maxwell distribution is valid for thermal equilibrium and in this case $b = (kT)^{-1}$, where k is the Boltzmann constant and T the absolute temperature of the system. There is no thermal equilibrium in a sputtering process and no equilibrium temperature can be defined in this case. Using (4) as an energy distribution function one obtains for the average particle energy:

$$E_{av2} \cong \frac{\int\limits_0^\infty E \cdot F(E)\mathrm{d}E}{\int\limits_0^\infty F(E)\mathrm{d}E} = \frac{3}{2} E_b \tag{5}$$

in contrast to (3) in calculating (5) the upper limits of the integrals were extended to the infinity instead of E_0 as a further approximation. The two results (3) and (5) are rather different for the usual E_0 values.

Figure 1 shows the two distributions in a normalized form. The approximation is seen to be rather good for the maximum and for the half width of the distribution, but there are big differences between the two distributions as the energy E will be higher and higher.

The sputtered particles are mostly neutral, but a small fraction (10^{-2} to 10^{-6}) will be emitted as an ion. In calculating the probability of primary-ion-induced secondary ion emission, many authors tried to use Saha—Langmuir type or related equations [5—7]. The general problem of this thermodynamical approach is the temperature, since no "temperature" can be defined in this case, as it is well known, and the "quasi temperature" values to be set in are rather high.

An attempt to calculate an equivalent temperature T_e using the equipartition theorem and (3)

$$T_e = \frac{2}{3k} E_{av1} \tag{6}$$

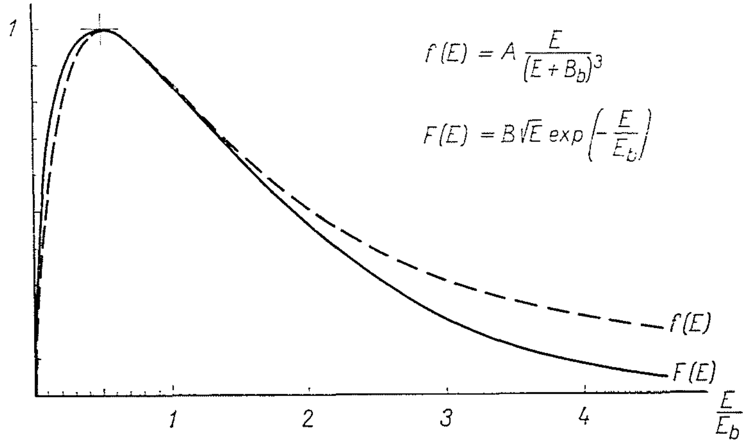

Fig. 1

is wrong in principle, because this relationship is intimately connected with a Maxwell—Boltzmann distribution. In a different case (e.g. fermion gas) (6) is not true. The general definition of the temperature in thermal equilibrium:

$$T = \left(\frac{\partial U}{\partial S}\right)_V \tag{7}$$

but using internal energy and entropy densities (7) can be extended to so-called linear thermodynamics e.g. to a stationary particle transport. The local thermal equilibrium (LTE) supposed even in (7) is, however, questionable in this case sputtering being a stationary particle source only in a time average [4].

On the other hand, assuming a stationary particle source model with energy distribution function (1) an equivalent "temperature" can be defined using (1) and (7) as follows.

Let us normalize (1), i.e.

$$\int_0^{E_0} A \frac{E}{(E + E_b)^3} \mathrm{d}E = 1 \tag{8}$$

then

$$A = 2E_b \left(\frac{1 + x_0}{x_0}\right)^2 \tag{9}$$

where

$$x_0 \equiv \frac{E_0}{E_b} \tag{10}$$

The internal energy density U can be obtained now as in (2). The precise result is:

$$U = NE_b \left[\left(\frac{1 + x_0}{x_0}\right)^2 \cdot 2 \cdot \ln (1 + x_0) - 3 - \frac{2}{x_0}\right] \tag{11}$$

in contrast to (3) where the terms with x_0^{-1} have been neglected and N is the number per second of the emitted particles.

Defining the entropy density by Boltzmann's formula in continuous approximation in the phase space and using (1):

$$S = - kN \int \Phi \ln \Phi \, \mathrm{d}\tau \tag{12}$$

where

$$\Phi = C \frac{\sqrt{E}}{(E + E_b)^3} \tag{13}$$

while

$$\mathrm{d}\tau = d^3\bar{r} d^3\bar{p} = d^3\bar{r}\, 2\pi\, m^{3/2} \sqrt{E}\, \mathrm{d}E \tag{14}$$

(*m* is the mass of the emitted particle.)

The integral (12) can be calculated in closed form. We are giving here explicity only that part of the entropy density which depends on x_0:

$$S = -\frac{kN}{2}\left[3\ln\frac{1+x_0}{x_0} + \frac{10x_0-5}{x_0^2}\ln(1+x_0) - \frac{8x_0+5}{x_0}\right] + S_0 \qquad (15)$$

where S_0 contains the terms not depending on x_0.

Using (7)

$$T = \left(\frac{\partial U}{\partial S}\right)_V = \frac{\left(\frac{\partial U}{\partial x_0}\right)_V}{\left(\frac{\partial S}{\partial x_0}\right)_V} \qquad (16)$$

so by (11) and (14)

$$T_0 = \frac{4E_b}{k}\,\frac{1 - \frac{x_0(2+x_0)}{2(1+x_0)\ln(1+x_0)}}{\left(\frac{x_0}{1+x_0}\right)^2\frac{6}{\ln(1+x_0)} - 5} \qquad (17)$$

In the case of $x_0 \gg 1$ in good approximation:

$$T_0 = 0.8\frac{E_b}{k}\,\frac{0{,}5\,x_0 - \ln x_0}{\ln x_0 - 1{,}2}\,. \qquad (18)$$

Comparing this with (4) and (6), obviously:

$$\frac{E_b}{k} < T_e < T_0 \qquad (19)$$

Actually (18) gives rather high temperature values, e.g. for $x_0 = 100$; $T_0 \approx 8E_b/k > 10^4\,°\mathrm{K}$, while $T_e \approx 6E_b/k$ in this case.

It has to be pointed out that the above calculations used a stationary model particle source, with an energy distribution function (1). Neither this procedure means that one could define a temperature in sputtering. We only wanted to show, that thermodynamical approach, as the Saha—Langmuir and related equations, to a case with no Maxwell distribution requires extra care of the concept "temperature".

Summary

The energy distribution of the sputtered atoms can be approximated by a Maxwell-type form in certain energy regions using the surface binding energy instead of temperature, as a fitting parameter. A temperature in sputtering cannot be defined although often thermo-

dynamical approach to some related problems has been used in the literature and rather high effective "temperature" values suggested. Assuming an ideal particle source model with the energy distribution of the sputtering, inner energy and entropy densities can be defined and an equivalent temperature calculated for the model.

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