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Short communication

Calculation of the surface binding energy for ion sputtered particles

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Abstract

In this paper, we consider a simple model, based on the electronegativity concept, which makes it possible to calculate the surface binding energy of any particles, sputtered from a solid surface by ion bombardment. The model contains empirical equations for calculation of "ionic" and "covalent" parts of the binding energy happened between a surface atom and its close neighbors. The model is strongly desirable in the case of the ion sputtering of any strong electronegative (C, N, O, F, Cl, etc.) or electropositive elements (alkali metals, rare earth elements) from semiconductor surfaces, when the strong ionic binding between these elements and the surface atoms can be estimated.

Keywords: Surface binding energy; Electronegativity; Sublimation energy; Ion sputtering

1. Introduction

The surface binding energy (SBE) is defined here as the energy, which is necessary to apply in order to remove an atom from the top surface layer in vacuum during the ion sputtering process. It is a very important parameter characterizing the ion sputtering process. Indeed, the sputtering yield of any target is inverse proportional to its SBE. It is known that the ion sputtering of multi-element target leads to the preferential sputtering of the elements. So, the surface concentration of the elements after ion sputtering differs from the bulk composition. Again, the final surface composition is defined in a great extent by the SBE of the elements. Any theoretical model, as well as any computer code, describing the ion sputtering process, uses the SBE. According with the Zigmund–Thompson model [1], for example, the energy distribution of sputtered particles is defined as follows:

$$\frac{\mathrm{d}N(E)}{\mathrm{d}E} \approx \frac{E}{(E + E_{\mathrm{bind}})^3}\cos(\vartheta), \qquad (1)$$

where E_{bind} is the SBE, and ϑ the emission angle of the sputtered particles. From Eq. (1), the maximum in the energy distribution is reached at the $E_{\mathrm{bind}}/2$ and can be found from experimentally measured energy distributions of sputtered atoms. Unfortunately, the authors don't know any publication devoted to experimental measurements of the SBE. Moreover, despite wide applications of the SBE, there is not still a model, which predicts the surface binding energy for different pairs: matrix–element and for any practical regimes of

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the ion sputtering. In most cases, theoreticians and analysts use the sublimation energy (SE) of elements as the SBE in their estimations. This approach looks quite reasonable in the case of the ion sputtering of matrix elements. However, using the sublimation energy for any low concentration dopant is not a good way. That is true especially in the case of strong electronegative elements like O, C, F, Cl, etc. and for strong electropositive elements like Cs, Na, K, Ba, etc. In these cases a strong ionic bond can appear between these elements and matrix atoms located in the top surface layer. As an illustrating example we can mention the binding energy of Cs atoms on Si(1 1 1)-(7 × 7) surface: 1.64 eV [2], and the sublimation energy of cesium, which is two times lower: 0.812 eV.

In this work, we considered a simple empirical model for SBE calculation, based on the electronegativity concept, developed by Pauling [3] and improved by his followers [4].

2. Basic estimations and model description

First of all we are going to describe some estimation, which support our model:

- We have limited our consideration by the case of the linear collision cascade regime of the ion sputtering.
- We considered the ion sputtering of pure mono (Si and Ge) and binary (III–V, II–VI) semiconductors.These two limitations correlate with SIMS (SNMS) analysis of dopants and contamination in the noted semiconductors:
- It is very important to notice that the ion sputtering of semiconductors is accompanied by an amorphization of a near surface layer. It is well known that amorphization of crystalline silicon happens under ion bombardment with doses of around 10^{15} ion/cm^2. Under the typical SIMS regimes, provided with modern instruments, this dose can be reached after approximately 2–3 s after start of the ion sputtering. In other worlds, all SIMS studies are performed for amorphized top surface layers. Taking that into account we excluded any crystal effect from our consideration and estimated our sputtering target as a molecular compound, where the SBE of a sputtered atom can be found as the binding energy between this atom and its closest neighbor in the first monolayer.

For example, the SBE of an element X (with low concentration) in Si can be found as the binding energy between X and the closest Si atom. The influence of other close Si atoms can be taken into account by special empirical approximations (see below). Of course, the estimation is quite rough, but it seems to be a more realistic approximation for calculation of the real surface binding energy in the noticed before cases, than the sublimation energy.

Then we considered a model, based on the empirical electronegativity concept, suggested by Pauling [3] and improved for hetero-atomic binding by Sanderson [4]. Pauling estimated that each atom does contribute to the covalent part of its bond energy in proportion to its homo-nuclear single covalent bond energy. Following that, we can separate contributions of the ionic and covalent binding energies and calculate them independently from different estimations. According to this approach, the binding energy of hetero-molecules can be calculated as the sum of the covalent binding energy $E_c(A-B)$ and the ionic binding energy $E_i(A-B)$ with corresponding weighting coefficients t_j [4]:

$$E_{\text{bind}}(A-B) = t_c E_c(A-B) + t_i E_i(A-B), \tag{2}$$

where $t_i + t_c = 1$.

The covalent binding energy term can be found as the geometric average of the covalent binding energies of interacting atoms, which they have in their homonuclear molecules (A–A and B–B):

$$E_c(A-B) = \sqrt{E_c(A-A)E_c(B-B)} \tag{3}$$

Note, that these energies are well known for many molecules (see for example [5]). The well-known Coulomb law can find the term for ionic binding energy,

$$E_i = \frac{\Delta q e^2}{d} \tag{4}$$

where e is the electron charge, Δq the partial charge of interacting particle (or ionicity of the binding), and d the inter-atomic distance between A and B atoms. In the first approximation d can be found as the sum of covalent radii of the binding atoms.