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Letter to the Editor

LATTICE LOCATION CALCULATION OF ELEMENTS IMPLANTED IN Si BY MIEDEMA PARAMETERS

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Fitting parameters for site energy difference expression of Miedema coordinates has been determined for Si.

Since Miedema et al. [1] have determined the relevant parameters for calculating the heat of mixing in binary alloys, different uses of the parameters have been published [2,3,7]. One important point made by Kaufmann et al. [4] refers to ion implantation. According to this, the values determined by Miedema contain information not only about equilibrium alloying, but more generally on metastable lattice location. In the case of a Be host, where ballistic effects are not important because of the large mass ratio, they could distinguish between different lattice locations by the sign of a simple second degree expression for the Miedema coordinates:

$$N^{si} = \sum_{i,j=1}^{2} a_{ij} x_i x_j + \sum_{i=1}^{2} b_i x_i + c, \qquad (1)$$

where N^{si} is the site energy difference of substitutional–interstitial lattice location,

$$x_1 = \mu(\text{host}) - \mu(\text{A}),$$
$$x_2 = n_{WS}^{1/3}(\text{host}) - n_{WS}^{1/3}(\text{A}). \qquad (2)$$

μ is the chemical potential and n_{WS} the electron density at the boundary of the WS cell of atoms A. We show in this letter that a similar separation and fitting procedure can be done in the case of a Si host.

Using recent work on lattice location of implanted heavy elements in Si at RT and 2–3 keV by Frerichs and Kalbitzer [5] we separated the 90% substitutional IV/A, V/A and the 60% tetrahedral elements quite clearly (fig. 1) despite the relative importance of ballistics and diffusion speed difference in the case of a Si host.

While Frerichs and Kalbitzer concluded that chemical effects govern by and large the selection of lattice sites, Antoncik [6] has attempted to understand the "fate" of implanted elements in silicon from all groups of the periodic system on the basis of s–p valence bonds. We found that the parameters of Miedema, which have been successfully applied in the case of a Be host, and the kinetical effects together give a good interpretation of experiments for implanted elements in [5] and for other well-known materials like Ga, As and Si in silicon.

We neglected the 50% substitutional III/A elements although they also lie near the encircled zone of substitutionals. Anomalies Ag and Hg at substitutional position elements U, Be, Pu at tetrahedral sites can be interpreted by the large mass ratio to Si, which causes large Frenkel pair separation following the cascade process.

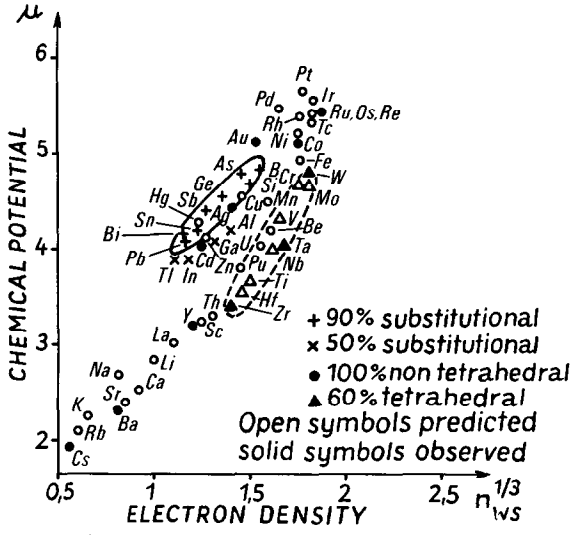

Fig. 1. Miedema plot of silicon with different elements. Elements of over 90% substitutionality are encircled. The dashed line is a fitted curve to approximate the region of experimentally tetrahedral elements. Anomalies of Ag, Hg or Be, U and Pu might be connected with large mass ratios to silicon and the uncertainty of Miedema parameters.

Table 1
Fitted coefficients to Miedema coordinates for Si

a_{11}	$a_{12}+a_{21}$	a_{22}	$2b_1$	$2b_2$	c
−17.138	53.3	−55.864	2.51	−11.424	0.07683

The fitting parameters a_{ij}, b_i, c to substitutional–interstitial site energy differences are tabulated in table 1.

With these parameters the boundaries of substitutional site regions are found as shown in fig. 1. Moreover, as Chelikowsky pointed out [8], they not only bare fitting values, but are correlated to shear elastic contants of the host lattice. Therefore, they should also account for the site energy differences of impurities in Si. Although the a_{ij}, b_i, c coefficients are probably not unique, the site energy differences (1) produced by them, seem to be reasonable.

The tetrahedral region can be separated by a second order expansion of x_1, x_2 too, which either can determine a closed elliptic or an open hyperbolic contour on the Miedema space.

As a conclusion, it was shown that Miedema parameters and Miedema's representation of metallurgical data is basically valid for silicon and thus site energy differences, diffusion of Frenkel pairs etc can be calculated on this basis as will be shown in another paper.

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