

CHANGES OF THE LATTICE PARAMETER IN Al 3d ALLOYS

M. Očko and E. Babić

TVA KoV JNA 256, Zagreb

Institut za fiziku Sveučilišta, Zagreb

Recent measurements of the lattice parameter of AlSc system¹⁾ have shown that the change of the lattice parameter in Al 3d alloys is influenced not only by the redistribution of the charge on impurity site but also by the difference in the period of Al and impurity. Comparing the experimental results (first column in Table I) with the theoretical calculations²⁾ based on virtual bound state (v.b.s.) picture (third column in Table I) one can see that: i) for AlSc system theory predicts a negative change in lattice parameter while experiment gives a positive one, ii) for other systems the theoretical results are up to a factor of ten bigger than the experimental ones, iii) these difference is bigger for the elements with lower atomic number.

To our opinion this discrepancy is primarily caused by neglecting the difference in period of Al and transition metal atom. Bletny³⁾ suggested that AlSc system could give proper correction for this effect since both Al and Sc have three electrons in the outer shells. However this correction does not improve significantly the agreement between the theory and experiment. The reason for that lies in the fact that the charge of the nuclei with higher atomic number is higher while the number of the electrons which form the "hard core" remains the same. Therefore this correction should change the atomic number but the calculation of this effect is difficult.

We propose the following empirical method to separate the effect of v.b.s. from the total change in the lattice parameter. We calculate the relative difference in atomic radii with respect to Al for the elements just in front and after 3d series (Ca and Zn) and assume that linear interpolation between these two points gives relative change in the lattice parameter for a given impurity without the v.b.s. contribution. By subtracting interpola-

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$\frac{1}{a} \frac{da}{dC}$	Ref.	Measured	Corrected	Theory	$\frac{\text{Theory}}{\text{Corrected}}$
Sc	1	+0.122	-0.216	-0.298	1.33
Ti	6	-0.199	-0.407	-0.546	1.30
V	6	-0.130	-0.387	-0.652	1.62
Cr	6	-0.170	-0.386	-0.976	2.44
Mn	6	-0.178	-0.354	-0.816	2.21
Fe	3	-0.130	-0.526	-0.587	2.18
Co	3	-0.105	-0.199	-0.292	1.47
Ni	3	-0.044	-0.097	-0.046	0.46
Cu	3	-0.125	-0.121	-0.175	1.38

ted values from our data we obtain approximately the effect of v.b.s. parameter which can be compared with theory⁴⁾.

Second column of Table I gives the corrected experimental data ("the experimental v.b.s.effect") and the last column gives the ratio of the theory with experiment. One can see that this ratio is still rather big for AlCr, AlMn and AlFe alloys i.e. for the impurities with about half-filled d-shell. This discrepancy can be explained by the attenuation of the charge oscillations near the impurity. The NMR experiments⁵⁾ on AlCr, AlMn and AlFe have shown that, due to strong attenuation, the charge oscillations cannot be described by the asymptotic expression^{2,3)}. Such attenuation was not observed for nonmagnetic impurities Sc,Ti,V etc. Therefore one can conclude that in AlCr, AlMn and AlFe systems the electric field which acts on Al atoms would be weaker for about a factor of two causing correspondingly smaller change of the lattice parameter. Thus the ratio between theoretical and experimental values becomes practically constant and about 1-1.5. Such a good agreement between the theory and the experiment indicates the correctness of our interpolation method.

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