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VACANCY RESISTIVITY DEPENDENCE ON LATTICE PARAMETER CHANGE IN PURE RAPIDLY QUENCHED ALUMINIUM SAMPLES

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Introduction

We begin our study of vacancies in URQ aluminium by correlating vacancy concentration obtained by different methods i.e. X-ray measurements and electrical measurements. It is well known that a large number of vacancies in material alters the lattice parameter and electrical resistivity. First we will sketch briefly some theoretical predictions on the electronic structure change by immersing point defects into the conduction electron gas which we consider for simplicity to be a free electron gas.

Theory

Now, let a point defect with a total charge of Ze be introduced into the free electron gas. The electrons become polarized around this charge and screen it so that the system becomes neutral on a macroscopic scale.

Let V(r) be the perturbing potential i.e. the Coulomb part of the point charge together with its screening charge, V(r) satisfies Poisson's equation

$$\Delta V(r) = 4\pi \left(n(r) - \Delta\varrho(r) \right)$$

where n(r) is the electronic density without the perturbation, and $\Delta\varrho(r)$ is the screening charge density. From the Fourier transforms of the last equation and by means of a static dielectric constant we obtain the total charge density induced by the presence of the point charge in the electron gas (1)

$$\Delta\varrho(r) = \frac{1}{(2\pi)^3} \int \left[\frac{1}{\varepsilon(k,0)} - 1 \right] n(k)\, e^{i\vec{k}\vec{r}}\, d^3k$$

We see that the screening properties depend on the dielectric constant of the non-interacting electron gas. We can calculate $\varepsilon(\kappa, \omega)$ in various approximations (2). The Hartree approximation gives the correct result, i.e. total screening charge equals Z, finite electronic density at the origin and the long range oscillations in the electronic density.

Using the assumption that the vacancies cause long range oscillations in the electronic density of the shape $\Delta\rho(r) \approx \frac{\cos \kappa r}{r^3}$, we can calculate the corresponding electric force which acting on the nearest neighbours causes the change in lattice parameter given by (3)

$$\frac{\Delta a}{a c_v} = (1+\varepsilon) \chi n r_0 F(r_0) / 9\Omega$$

where ε is a numerical factor, χ the compressibility of aluminium, n the number of the nearest neighbour atoms, r_0 their mean distance, and $F(r_0)$ the electric force. In the case of vacancies in aluminium we obtain $\frac{\Delta a}{a c_v} = 0.1$

Experimental procedure

In our experiments we prepared samples of pure Al by URQ from the melt, to obtain considerable increase in vacancy concentration. The Al was 99.997% pure, with resistance ratio at room temperature and that at liquid He temperature being $\frac{R_{295}}{R_{4,2}} \approx 900$ before quenching. We selected several samples for every quenching speed and we measured their room temperature resistance R_{295} as well as their resistance at liquid helium temperature. From this data residual resistivity ratio $\rho = \frac{R_{4'2}}{R_{295} - R_{4'2}}$ was calculated. By multiplying ρ with pure Al resistivity at room temperature, the residual resistivity of the sample caused by vacancies is obtained.

Immediately following the resistance measurements the samples were prepared to obtain Debye-Scherrer diagrams. Some samples which were subsequently annealed 1 hr at 350°C have shown the lattice parameter of the original Al i.e. $a = 4{,}0495$ Å. Thus we preclude the possibility that the lattice parameter had been altered by the inclusion of impurities during sample preparation.

Results and discussion

The dependence of residual resistivity of our samples on relative lattice parameter change is shown on Fig.1.

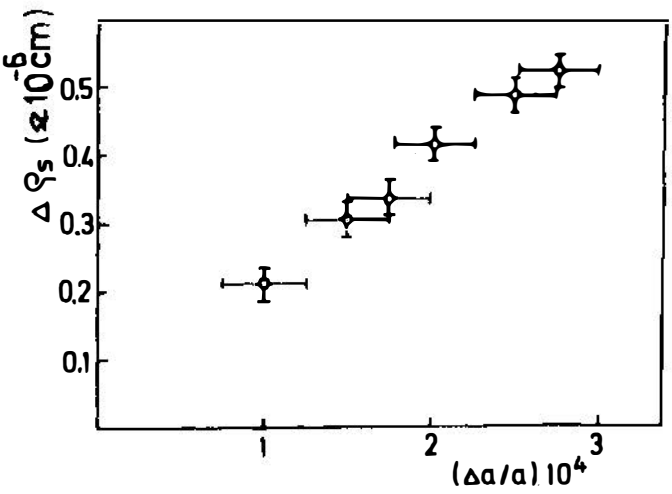

FIG. 1

Residual resistivity ρ versus lattice parameter change $\frac{\Delta a}{a}$

If we assume that the residual resistivity is caused by vacancies, we can find their concentration knowing that the specific resistance for an atomic percent of vacancies is $\rho_v = 3\,\mu\Omega$cm . The results of our measurements are shown on Table 1.

As expected, the values of vacancy concentrations obtained in this manner are somewhat too large but are still within reasonable limit considering the very coarse assumptions made in this calculation.. The last column shows the ratio of the two vacancy concentrations obtained by electrical and X-ray measurements, for samples quenched at different speeds.

If we take that the vacancy concentrations obtained on the basis of electrical measurements are accurate, we would obtain the same result by taking $\Delta a/a.c_v = -0{,}15$.

TABLE I

Vacancy resistivity is denoted by $\Delta\rho_1$, vacancy concentration as calculated from resistance measurements is given as $C_v(\rho)$. The lattice parameter changes are denoted by Δa , while vacancy concentrations $C_v(a)$ are calculated taking $\Delta a/a c_v = -0.1$.

Sample	$\Delta\rho_1$ ($\mu\Omega$cm)	$C_v(\rho)$	$-\Delta a$ (Å)	$C_v(a)$	$\frac{C_v(a)}{C_v(\rho)}$
1	0,53	$1,8 \cdot 10^{-3}$	$11 \cdot 10^{-4}$	$2,7\ 10^{-3}$	1,5
2	0,49	$1,6 \cdot 10^{-3}$	$10 \cdot 10^{-4}$	$2,5\ 10^{-3}$	1,6
3	0,42	$1,4 \cdot 10^{-3}$	$8 \cdot 10^{-4}$	$2,0\ 10^{-3}$	1,4
4	0,34	$1,1 \cdot 10^{-3}$	$7 \cdot 10^{-4}$	$1,7\ 10^{-3}$	1,5
5	0,31	$1,0 \cdot 10^{-3}$	$6 \cdot 10^{-4}$	$1,5\ 10^{-3}$	1,5
6	0,22	$0,7 \cdot 10^{-3}$	$4 \cdot 10^{-4}$	$1,0\ 10^{-3}$	1,4

A more complete picture will perhaps be obtained when an annealing study is made on the same samples.

Acknowledgements

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References

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DISCUSSION :

K. Mukherjee : When we have isolated single vacancies in thermal equilibrium, such as in the experiments of Fader and Nowick and Balluffi and Simmons, then the uniform lattice dilatation (as calculated by Eshelby) is proportional to vacancy concentration. However in a quenched system, when you have experimental evidence that relatively large vacancy clusters are present, I do not believe that a one to one correlation beetween Δa and vacancy concentration holds.

I. Zorić : Our experimental results confirm a one to one correlation beetwen Δa and vacancy concentration.

E. Nagy : What kind of free electron gas dielectric constant have you used, TF, Hartree or RPA ?

I. Zorić : Hartree approximation.