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The positron–dislocation interaction studied in deformed zinc single crystals

Shi Dan†, L Y Xiong†‡ and C W Lung†‡

† Institute of Metal Research, Academia Sinica, Shenyang 110015, People's Republic of China

‡ International Centre for Materials Physics, Academia Sinica, Shenyang 110015, People's Republic of China

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Abstract. The pyramidal dislocations and parallel basal dislocations induced from the deformation with compressive loading normal to the (0001) plane and to the $(10\bar{1}2)$ plane of the Zn single-crystal specimen are observed by TEM. The positron lifetime experiments for the samples measured at 100 K yield two different trapping lifetimes. It is found that the lifetime τ_d of positrons trapped and annihilated in basal dislocations lines increases by about 20% compared with that in bulk ($\tau_d = 177 \pm 2$ ps) and it is shown that a positron would be trapped in deeper traps (jogs) via the dislocation when the jog concentration along it is sufficiently high, with the annihilation lifetime close to that in a monovacancy. The intensities of the two trapping components decrease evidently with increase in temperature increasing to room temperature. The difference between positron–vacancy and positron–dislocation interactions are discussed.

1. Introduction

The positron annihilation method has proved useful in studying the electronic structure of lattice defects (West 1973, Hautojarvi 1979). Many investigations on the problem of the positron–dislocation interaction have been undertaken in deformed metals. This problem is still under active discussion. Most positron lifetime experiments on metals containing dislocations have yielded lifetime values for the trapped positron close to those for monovacancies. In the interpretation of such results, it is natural to assume that the long lifetimes result from positron trapping and annihilation along dislocation lines. By this means, Arponen *et al* (1973) have obtained a positron–dislocation binding energy of about 3 eV in Al. Martin and Paetsch (1972) calculated the positron binding energy based on pairwise interaction between the positron and metal ions. The resulting binding energy varied between 0 and 0.1 eV; the trapping lifetime is almost equal to the bulk lifetime.

An alternative model describing the positron–dislocation interaction has been proposed by Doyama and Cotterill (1979). They suggested that a dislocation line itself might be too narrow to localise the positron, while a jog and/or vacancy attached to the dislocation line could provide sufficient space. On the basis of this idea, Smedskjaer *et al* (1980) regarded a dislocation as a stepping stone to even deeper traps and calculated the temperature dependence of the detrapping rate from the dislocation line.

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Recently some positron lifetime measurements on deformed Zn crystals (Hidalgo *et al* 1986a, b, 1987) have been treated with the model suggested by Smedskjaer *et al* (1980). Hidalgo *et al* (1987) concluded that thermally activated positron detrapping would take place above 120 K. In their experiments, the jog concentration along a dislocation line is so high that they obtained only the parameters for positrons annihilating in jogs. As the basal slip system $\langle 11\bar{2}0\rangle\{0001\}$ is far easier to operate than other secondary slip systems in the deformation of Zn single crystals, Lavrent'yev and Salita (1979) and Lavrent'yev and Nikiforenke (1980) have pointed out that only the basal dislocation would be produced on operation of the first slip system by use of the shear direction $\langle 11\bar{2}0\rangle$. Because of the stability of basal dislocations, it is difficult to form a jog along the dislocation line (Friedel 1964). These conclusions make Zn single crystals a suitable system for studying the problem of the positron–dislocation interaction directly. For this purpose, we have performed positron lifetime measurements and transmission electron microscopy (TEM) studies on deformed Zn single crystals. In § 2 the experimental details are given; the experimental results are reported and discussed in § 3; the conclusions are given in § 4.

2. Experimental details

A single-crystal rod of diameter 20 mm was grown from Zn of purity 99.999% by the Bridgman method. Slices of the sample with a thickness of 2 mm were obtained by spark cutting, which was carried out in such a way that the cutting planes were parallel to the (0001) and $(10\bar{1}2)$ planes. The samples were annealed in vacuum at 650 K for 24 h and furnace cooled; then they were chemically polished with a HCl solution to remove the surface contaminants. The initial density of basal dislocations in the $\langle 11\bar{2}0\rangle\{0001\}$ slip system is about 10^5 cm^{-2}, after the above treatments, and that of pyramidal dislocations in secondary slip systems about 10^3 cm^{-2}. The samples were deformed with compressive loading perpendicular to the cutting planes at room temperature. The thickness reduction of sample Zn–A with its cutting plane parallel to the (0001) plane is about 7%; for sample Zn–B with the cutting plane parallel to $(10\bar{1}2)$, the thickness reduction is about 4%.

Positron lifetime spectra were obtained using a conventional fast-slow coincidence system made by Ortec, with an instrumental resolution (FWHM) of 302 ps. The samples were measured at 100 and 300 K. A positron source was made by evaporating 2.6×10^5 Bq of aqueous ^{22}NaCl solution onto a polyester foil. The fraction of positrons annihilating in salt and polyester foil was separated from the positron lifetime spectra for well annealed Zn (in which only one component is expected as a result of bulk annihilation at different temperatures. The values of the long-lifetime components associated with decay at the source surface are about 340 ps, and the corresponding intensities about 10%. The lifetime spectra obtained in our experiments are analysed with the positron extended program (Kirkegaard and Eldrup 1974).

After the positron lifetime spectra had been measured, thin-foil specimens of the deformed samples for TEM were prepared by the electrochemical method using an electrolyte consisting of 30% Cr_2O_3 and 70% H_2O, to avoid inducing new dislocations. The bright-field images of dislocations in the specimen were obtained with a JEOL-200CX electron microscope.

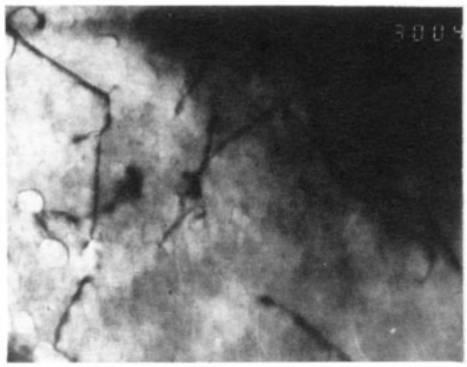

Figure 1. The bright-field image of dislocations in sample Zn-A. (Magnification, 30 000×.)

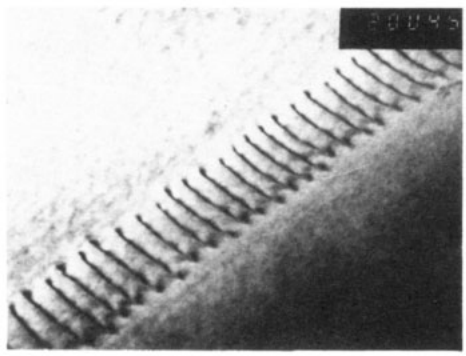

Figure 2. The bright-field image of a group of parallel dislocations in sample Zn-B. (Magnification, 20 000×.)

3. Results and discussion

Because the loading direction is normal to the base plane for sample Zn-A, pyramidal dislocations are induced by second-order slip systems $\langle 11\bar{2}3\rangle$ $\{11\bar{2}2\}$. The bright-field image of these dislocations is shown in figure 1. As the forest dislocations become tangled with each other and penetrate the base plane to form jogs at their intersections easily (Friedel 1964), the jogs along the dislocations should be quite dense. Figure 2 is the TEM bright-field image for a group of parallel dislocations in sample Zn-B. Because the loading axis is normal to the $(10\bar{1}2)$ plane which is at an angle of 43° with the (0001) plane, according to the Schmid rule, the greatest shear stress is almost in the $\langle 11\bar{2}0\rangle$ direction, and only the basal slip system would be operating (Lavrent'yev and Salita 1979). We infer that figure 2 is the image of basal dislocations. It can be estimated from figure 2 that the dislocation density is about $10^{10}\,\mathrm{cm}^{-2}$, and the jog concentration along them is less than $10^{-3}\,\mathrm{nm}^{-1}$. Because of the mobility of monovacancies in Zn (Schumacher 1970), the existence of monovacancies could be ruled out (Hidalgo *et al* 1986b), and only dislocation-type defects are considered for positron trapping in the deformed Zn samples.

Table 1. The results of a free analysis with two components for $T = 100$ K.

Sample	τ_1 (ps)	I_1 (%)	τ_2 (ps)	I_2 (%)	$\bar{\tau}$ (ps)
Zn-A	100 ± 4	36	227 ± 3	64	181
Zn-B	96 ± 4	22	177 ± 2	78	160

When the positron lifetime spectra for samples Zn-A and Zn-B are fitted with a single component, it is found that the values of positron lifetime are about 30 ps and 10 ps, respectively, more than the bulk lifetime τ_b of 150 ps obtained from measurements on a well annealed Zn sample at 100 K. The variations in the fit for the deformed samples are over 1.68. The results of a free analysis with two components for the lifetime spectra are listed in table 1, and the variations decrease to 1.18. The longer lifetimes in table 1 are labelled as τ_{2A} for sample Zn-A and τ_{2B} for sample Zn-B. The difference between them is about 50 ps, and τ_{2A} is close to the lifetime value τ_V of 240 ps for a positron annihilated in a vacancy. As mentioned above, both the two longer lifetimes would result from positrons trapped and annihilated in dislocation-type defects, and it is difficult to understand that there are two different trapping lifetimes for a single type of dislocation. From the discussion of figures 1 and 2, it can be seen that the jog concentrations along forest dislocations are far higher than those along basal dislocations. The above results would be explained well by the model for describing a positron–dislocation interaction on the assumption that a positron is trapped in even deeper traps via the dislocation line, if the jogs along it are sufficiently dense. The lifetimes that τ_{2A} and τ_{2B} represent will be emphasised in the following discussion.

In the present work, it is appropriate to assume that the positron detrapping rate from a dislocation line at 100 K is so low that it can be ignored in comparison with the annihilation rate in the dislocation. This is in agreement with the results obtained by Hidalgo *et al* (1987). On the basis of this hypothesis, an interpretation of a two-defect trapping model without detrapping can be described as in figure 3. η and η' represent the transition rates which are proportional to the jog concentration along a dislocation, and κ is the trapping rate of free positrons at a dislocation line. $\lambda_{b'}$, λ_d and λ_j are the positron decay rates in the bulk, dislocation lines and jogs, respectively.

For sample Zn-A, we believe that $\eta \gg \lambda_d$. The probability A_j that a positron will be trapped and annihilated in a jog can be obtained from the steady-state equation given by Smedskjaer *et al* (1980):

$$A_j \simeq (\kappa + \eta')/(\lambda_b + \kappa + \eta').$$

It shows that most positrons trapped along a dislocation line will annihilate in jogs. τ_{2A} in table 1 is the lifetime of positrons annihilated in jogs.

As the jog concentrations along basal dislocations in sample Zn-B are far lower than those in sample Zn-A, we speculate that $\lambda_d + \eta \leqslant \lambda_b + \kappa$ for sample Zn-B. The rate equations can be established as

$$\begin{aligned} \dot{n}_b &= -(\lambda_b + \kappa + \eta')n_b \\ \dot{n}_d &= -(\lambda_d + \eta)n_d + \kappa n_b \\ \dot{n}_j &= -\lambda_j n_j + \eta n_d + \eta' n_b. \end{aligned} \tag{1}$$

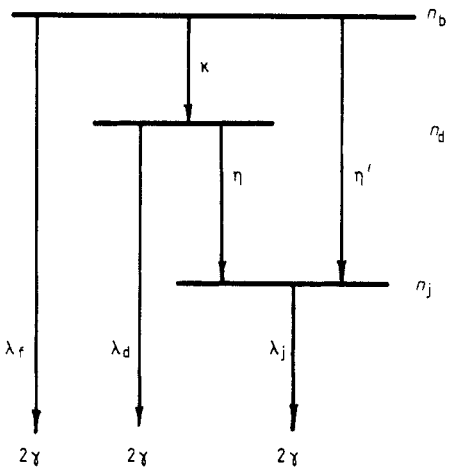

Figure 3. Decay scheme for two types of defect without detrapping from the dislocation line (n_b, rate in the bulk; n_d, rate at a dislocation; n_j, rate at a point defect).

In general, the transition rate η' can be neglected, as $\eta' \ll \eta$ (Smedskjaer *et al* 1980). A positron lifetime spectrum is given by

$$S(t) = \lambda_b n_b + \lambda_d n_d + \lambda_j n_j = \sum_{i=1}^{3} I_i \lambda_i \exp(-\lambda_i t) \tag{2}$$

where $\lambda_1 = \lambda_b + \kappa$, $\lambda_2 = \lambda_d + \eta$ and $\lambda_3 = \lambda_j$. The relative intensities I_i ($i = 1, 2, 3$) for the three annihilation components can be obtained from the solution of equation (1) and are given in the following equation:

$$I_2 = [\kappa/(\lambda_1 - \lambda_2)](\lambda_d - \lambda_3)/(\lambda_2 - \lambda_3) \qquad I_3 = [\kappa/(\lambda_1 - \lambda_3)][\eta/(\lambda_2 - \lambda_3)]$$
$$I_1 + I_2 + I_3 = 1. \tag{3}$$

On the assumption that the shortest component can be easily separated from the others, the longer lifetime τ_{2B} obtained experimentally should be identified with the mean lifetime of $\tau_2(\equiv 1/\lambda_2)$ and $\tau_3(\equiv 1/\lambda_3)$. Then we can write the expression for τ_{2B} as follows:

$$\tau_{2B} = (I_2\tau_2 + I_3\tau_3)/(I_2 + I_3)$$
$$= \tau_2[1 + \tau_3\eta(\lambda_1 - \lambda_2)/(\lambda_1 - \lambda_j - \eta)]. \tag{4}$$

τ_2 should be greater than $1.5\tau_1$; otherwise it would be difficult to separate τ_2 from the shortest component. Let $\tau_2 \geqslant 150$ ps, $\tau_1 = 96$ ps, $\tau_{2B} = 177$ ps and $\tau_3 = 227$ ps in equation (4); then $\eta \leqslant 1.05 \times 10^{-3}$ ps is obtained for sample Zn-B. We can easily obtain the lifetime value of a positron annihilated at basal dislocation lines from the expression for λ_2: $\tau_d = 177 \pm 2$ ps. This value is nearly 30 ps more than λ_b at 100 K.

The positron lifetime results of a free analysis with two components are listed in table 2 for the samples measured at 300 K. The mean lifetime of a positron annihilating in sample Zn-B is only 4 ps more than that in well annealed Zn, taking into account the change in τ_b with temperature, and we could not physically decompose any trapping component. In a well annealed Zn sample, we found experimentally that $\Delta\tau_b/\tau_b = 0.04$ between 100 and 300 K. For sample Zn-A, the value of τ_{2A} is almost independent of

Table 2. The results of a free analysis with two components for $T = 300$ K.

Sample	τ_1 (ps)	I_1 (%)	τ_2 (ps)	I_2 (%)	$\bar{\tau}$ (ps)
Zn-A	129 ± 3	50	210 ± 5	50	170
Zn-B	160	100	—	—	—

the sample temperature, but the component intensity decreases evidently. When the trapping process is transition limited, the trapping rate will be independent of sample temperature (Bergersen and Mcmullen 1977). We suggest that the decrease in intensity of longer-lifetime component as the temperature is raised is induced by the detrapping of the thermally activated positron from dislocation lines.

Xiong (1986, 1988) has defined a quantity γ as the open-space ratio of a dislocation core to a monovacancy in order to express the difference between the electron densities in these defects:

$$\gamma \equiv \Delta V_d / \Delta V_v \simeq (\lambda_b - \lambda_d)/(\lambda_b - \lambda_v). \tag{5}$$

With $\Delta V_d = V_b - V_d$, $\Delta V_v = V_b - V_v$, where V_b, V_d and V_v are the volume elements in which the same amount of electrons is involved in the bulk, in the dislocation core and in the monovacancy, respectively. Let $\lambda_f = 1/150\ \text{ps}^{-1}$, $\lambda_d = 1/177\ \text{ps}^{-1}$ and $\lambda_v = 1/240\ \text{ps}^{-1}$ in equation (5); one can obtain $\gamma \simeq 0.4$ for Zn. When it is taken into account that the enhancement factor for positron annihilation increases with decrease in electron density around a positron, then γ would be less than 0.4. This means that the electronic structure in the dislocation core is not similar to that in a monovacancy, and the positron–dislocation interaction could not be described by the model proposed by Arponen *et al* (1973), in which the ion density inside the dislocation core was set to zero. By means of this interpretation, the electrostatic part of the trapping potential would descend sharply, making it comparable with that calculated by Arponen *et al* (1973). Therefore the positron–dislocation binding energy should be lower than that for a vacancy. On the other hand, we have obtained that the positron lifetime τ_d due to trapping and annihilation in a basal dislocation line at 100 K is different from τ_b. This indicates that, if one calculates a rate of positron annihilation along a dislocation line, it would be useful to take the functions of both free electrons and core electrons in the dislocation core into account to fit the experimental results.

4. Conclusion

Deformed Zn single-crystal samples with compressive loading normal to the (0001) plane and to the $(10\bar{1}2)$ plane have been studied by means of positron lifetime measurements and TEM. It is demonstrated that when the jog concentration along a dislocation is sufficiently high, the positron–dislocation interaction can be described by the generalised model (Smedskjaer *et al* 1980) in which a dislocation acts as a stepping stone to even deeper traps (jogs) at $T = 100$ K and that, if the jog concentration is less than $10^{-3}\ \text{nm}^{-1}$, most of the positrons trapped along a dislocation line will be annihilated in it with a lifetime τ_d of 177 ± 2 ps. It is shown that a dislocation line itself is a weaker trap than a vacancy, but the positron annihilation parameters in it are different from those in bulk.

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