Study of the Mg-Cd system by positron annihilation methods

1998 J. Phys.: Condens. Matter 10 6573

(http://iopscience.iop.org/0953-8984/10/29/017)

J. Phys.: Condens. Matter **10** (1998) 6573–6584. Printed in the UK PII: S0953-8984(98)92021-5

Study of the Mg–Cd system by positron annihilation methods

E Dryzek†, J Kuriplach‡ and J Dryzek†

† Institute of Nuclear Physics, PL-31-342 Kraków, ul. Radzikowskiego 152, Poland

‡ Department of Low Temperature Physics, Charles University, V Holešovičkách 2, CZ-180 00 Prague, Czech Republic

Received 25 February 1998, in final form 20 April 1998

Abstract. The problem of preferential positron annihilation in binary alloys has not been satisfactorily solved in the past. We examine this effect experimentally in Mg–Cd alloys using the new technique of Doppler broadening measurements with background reduction which allows us to observe positron annihilation with core electrons. Conventional positron lifetime spectroscopy is applied as well. We measure the Doppler spectra and positron lifetimes for selected alloys in the whole concentration range of the Mg–Cd system. The analysis of experimental results is supported by theoretical calculations. The conclusion is given that a small positron preferential annihilation occurs at Mg sites. Besides, the temperature dependencies of the peak counting rate of the angular correlation curve are measured for several samples and the vacancy formation energies are established. In the case of Mg–20 at.% Cd alloy, the increase of the peak counting rate characteristic for generation of thermal vacancies shows a discontinuity close to the order–disorder transition temperature.

1. Introduction

Positron annihilation spectroscopy (PAS) is a suitable tool for studies of binary alloys. It can provide information, e.g., about their electronic structure, the presence of open volume defects, temperature induced structure changes, etc. It is worthwhile to mention that in binary alloys so-called preferential positron annihilation may occur [1]. If a positron is present in a lattice which contains two sorts of atom (say A and B), the rate characteristic for positron annihilation with an electron of an A atom may be higher than the rate in pure element A. Furthermore, if there is an 'enhancement' of positron annihilation at A sites, there should be a reduction of annihilation at B sites with respect to pure element B. This effect is then called preferential positron annihilation (PPA) at A sites. The PPA is a consequence of the fact that the positron interaction with atoms is different in the alloy and in the pure elements whose atoms constitute the alloy. This effect was not proved conclusively enough despite several experimental and theoretical papers. The PPA in binary alloys was theoretically considered by Stott and Kubica [1] who have found a strong preference of positron annihilation or 'affinity' of positrons to core electrons of atoms of one sort as compared to others. Nevertheless, an attempt at observing this effect made by Kubica *et al* [2] in the Li–Mg system supports only qualitatively the theoretical predictions. According to, Kubica *et al*, the results of angular correlations of two annihilation quanta and positron lifetime measurements for Li–Mg alloys indicated that annihilation in the Li-rich regions of alloys is preferred by positrons. The theoretical paper by Szotek *et al* [3] concluded that the PPA appears only in specific conditions which are not valid for a large group of binary alloys.

0953-8984/98/296573+12$19.50

Experimental positron annihilation studies were performed for several systems. In some cases (Ni–Cu [4], Ag–In [5], Co–Si [6]) a linear dependence of the positron annihilation rate on the alloy composition was observed. For other alloys (Pd–Cu [4], Pd–Au [7], Fe–Al [8]) deviations of the annihilation rate from a straight line were found. In order to make some conclusions concerning the PPA on the basis of an experiment, attention should be paid to the following points. Firstly, the dependence of the atomic volume of an alloy on its composition must be considered [8]. The reason is that the positron lifetime (and annihilation rate) is a function of this volume. Secondly, the crystal structure can also change with the composition. There is a possibility that two or more phases exist in a sample. These phases are separated by interfaces which can act as trapping sites for positrons. Generally, the positron studies of binary alloys require a detailed analysis of the phase diagram. Thirdly, in many cases the study of the PPA was performed on alloys whose components have similar electronic structures, so the detection of the PPA was difficult. Fourthly, the application of positron lifetime and/or one dimensional angular correlation techniques to the studies of the PPA does not bring satisfactory results. Both techniques are more sensitive to the positron annihilation with valence electrons than with core electrons. Conversely, the measurements of the Doppler broadening spectra can yield more information about the annihilation with core electrons.

In order to overcome most difficulties specified above, we have chosen the Mg–Cd system [9, 10]. Both Mg and Cd have hexagonal close packed structures, the lattice parameters of which are very similar. The atomic radii of both elements are also similar. Due to these similarities both metals show continuous mutual solubility in a wide range of concentrations at elevated temperatures. At room temperature three ordered phases exist: α' ($MgCd_3$), α'' (MgCd) and α''' (Mg_3Cd) with the approximate maximum composition ranges 68–75, 40–62 and 18–35 at.% Mg, respectively. Nevertheless, the core electronic structures of both metals differ fundamentally: a Cd atom contains d electrons which are not present in an Mg atom.

In our study we applied the measurements of the positron lifetime and the Doppler broadening of annihilation line with reduction of the background. The latter technique has been proved to be efficient in studies of positron annihilation with core electrons (see, e.g., [11]). In section 2 we present the sample preparation procedure and description of the apparatus. Subsection 3.1 contains the results and discussion of the Doppler broadening and positron lifetime measurements carried out on alloys with different Mg concentration. The experimental results were compared with the calculations based on the atomic superposition (ATSUP) [12] and *ab initio* self-consistent tight-binding linear muffin-tin orbital (TB–LMTO) [13] methods. Additionally, the temperature dependencies of the peak of the angular correlation curve for selected alloys are discussed in subsection 3.2.

2. Experimental details

2.1. Sample preparation

Mg–Cd alloys with 3.5, 7.8, 13.8, 20, 50 and 95 at.% of Cd content were prepared. Calculated amounts of Mg (99.5%) and Cd (5N) were melted under flux (25% $CaCl_2$, 58.5% KCl, 1.5% NaCl, 12.5% $BaCl_2$, 2.5% CaF_2). The samples were prepared in the form of discs about 1 mm thick and 8 mm in diameter and annealed in evacuated glass ampoules for 72 hours at temperatures about 100 °C lower than their liquidus temperatures, then slowly cooled to room temperature. The samples were checked by x-ray diffraction. In

the case of Mg-rich alloys the dependence of lattice parameters on Cd content [9] allowed us to determine the alloy composition more precisely. In the case of Mg–20 at.% Cd the Cd content was determined using the Rutherford backscattering technique. Before the positron annihilation measurements were taken the surface of the samples had been etched in a dilute nitric acid aqueous solution in order to remove any surface oxides.

2.2. Apparatus

The lifetime spectra were obtained using a conventional fast–fast lifetime spectrometer with NE111 plastic scintillators with a time resolution (FWHM) of 300 ps for the ^{22}Na energy window. Data were analysed using the computer program called LT [14]. In all the spectra corrected for the source and background only one lifetime component could be resolved.

Doppler broadening (DB) spectra were collected using a coincidence spectrometer composed of a HpGe detector with an energy resolution 1.24 keV interpolated at 511 keV and an NaI(Tl) scintillator detector. As a positron source we used 0.23 mCi activity of ^{22}Na enveloped in Kapton foil. The coincidence spectrometer has been described elsewhere in detail [15]. The peak to the background ratio achieved was about 600:1. After the background subtraction the spectra (i.e. right-hand sides of annihilation peak) were normalized to unity.

The temperature dependences of the coincidence counting rate at the peak of the angular correlation curve of annihilation quanta were measured using a long slit angular correlation spectrometer with optical resolution 3 mrad $\times$ 379 mrad. The sample, the ^{22}Na source and the heater were placed in a vacuum chamber under a pressure 10^{-2} Pa. The temperature was controlled and stabilized with an accuracy of $\pm 1\,^{\circ}$C. The measurement at each temperature took 2 h in order to achieve thermal equilibrium.

3. Results and discussion

3.1. The search for the PPA

The measured values of the positron bulk lifetime (τ_f) for Mg, Cd and selected phases of the Mg–Cd system are summarized in the second column of table 1. The next columns contain positron lifetime values calculated by the ATSUP and self-consistent TB–LMTO methods. In our calculations the enhancement factor and positron correlation potential [16] obtained within the generalized gradient approximation (GGA) were used (hereafter we will call such calculations GGA calculations and the corresponding computational scheme will be denoted as the GGA scheme). It can be seen from table 1 that a better coincidence with the

Table 1. The values of the bulk positron annihilation lifetime (in ps), for stoichometric phases of Mg–Cd alloys measured experimentally and calculated using the ATSUP and TB–LMTO methods (the GGA scheme was applied).

	Experimental value	ATSUP	TB–LMTO
Mg	225.9 ± 1.0	226.0	216.3
Mg_3Cd	207.4 ± 1.0	209.6	198.4
MgCd	201.8 ± 1.0	197.8	185.5
$MgCd_3$	—	189.1	175.8
Cd	187.5 ± 1.0	184.2	167.2

experiment was achieved when the ATSUP method was used. Surprisingly, the TB–LMTO method underestimated the positron lifetime in the case of Cd where the calculated value was about 20 ps lower than the measured one (cf also [17]). In the calculations we also used the approximation (for enhancement and positron potential) introduced by Boroński and Nieminen [18]; however the agreement between the theoretical and experimental values of the positron lifetime was not as good as in the case of the GGA scheme.

In table 1 we omitted the measured value of the bulk lifetime for $MgCd_3$. The measurements of the positron lifetime in several such samples exhibited only one lifetime component which was close to 212.8 ± 2 ps. The measurement of the x-ray diffraction in the samples revealed the coexistence of the α' phase ($MgCd_3$) and the small amount of the α phase (solid solution of Mg in Cd). The lifetime value obtained may be due to the annihilation of positrons trapped in structural vacancies or interfaces between phases which had not been removed during the long tempering of the samples.

Figure 1 presents the positron annihilation rate ($\lambda_f = 1/\tau_f$) as a nonlinear function of Cd content in the Mg–Cd alloys. This nonlinearity may indicate the presence of PPA. Nevertheless, it is known from the x-ray diffraction data [9, 10] and confirmed by our x-ray diffraction measurements that the atomic volume exhibits a nonnegligible dependency on the Cd content (x). This dependency can be approximated by the following formula: $V\ [\mathrm{nm}^3] = 2.3255\times10^{-2} - 0.0558\times10^{-3}x + 9.6682\times10^{-8}x^2 + 5.0119\times10^{-9}x^3 - 2.0559\times10^{-11}x^4$. The positron annihilation rate in the bulk is a function of the atomic volume (V) and the number of conduction electrons per atom (z). The following empirical formula was proposed by Seeger and Banhart [19]:

$$\lambda_f = \frac{1}{\tau_f[\mathrm{ns}]} = 2.004\left[\left(\frac{1.5394z}{V\ [\mathrm{nm}]}\right)^{0.81} + 1\right]. \tag{1}$$

Let us assume that for pure Mg, $z_{Mg} = 1.911$, pure Cd, $z_{Cd} = 2.629$ (these figures reproduce the experimental values of the positron lifetime from equation (1)) and for the $Mg_{1-x}Cd_x$

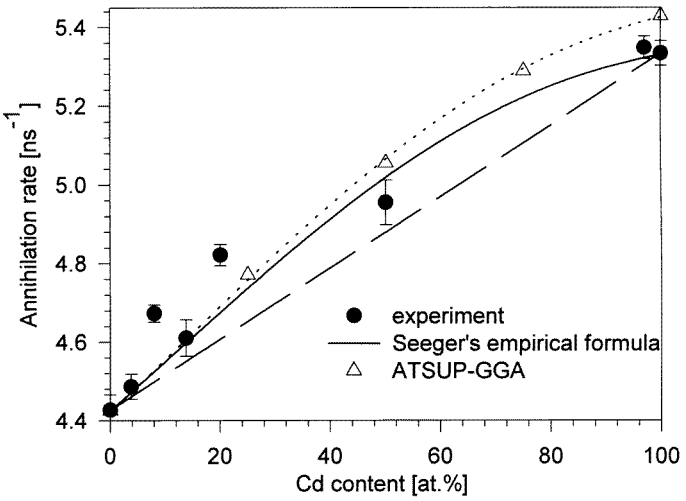

Figure 1. Experimental and theoretical annihilation rates as a function of Cd content in Mg–Cd alloys. The dashed line is straight. The solid line corresponds to the empirical formula (1). The open triangles represent the results of the ATSUP–GGA calculations given in table 1. The dotted line was obtained applying equation (1) to the theoretical values of annihilation rates.

alloy, $z = z_{Mg}(1-x)+z_{Cd}x$. If we put the formula for the atomic volume into equation (1), we obtain a dependency which is plotted as the solid line in figure 1. Therefore, the observed nonlinearity of the annihilation rate can be probably explained as a result of changes of the alloy atomic volume. A similar analysis performed for Fe–Al alloys also indicated that changes of the atomic volume were responsible for a nonlinear dependence of the positron annihilation rate on the alloy composition [8].

In order to find out whether PPA takes place in the Mg–Cd system, we performed the theoretical self-consistent calculations of the positron annihilation rate using the TB–LMTO method in bulk Mg, Mg_3Cd, MgCd, $MgCd_3$ and Cd neglecting changes of the atomic volume with the composition. This theoretical approach, first suggested in [8], may not exactly correspond to real conditions (volume) of alloys; nevertheless it allows us to evaluate quantitatively the PPA effect. We made two sets of calculations with atomic volumes fixed at values of Mg and Cd (to be sure that the conclusion does not depend on the volume chosen) and we calculated again the annihilation rates. On the basis of these calculations one can extract the positron annihilation rates with the Mg and Cd electrons separately. The results for the Cd atomic volume obtained using the GGA scheme (open circles) are summarized in figure 2. The partial annihilation rates for Cd (Mg) are located slightly below (above) the straight line. The straight lines would be valid in the case of no PPA. This allows us to draw a conclusion that positron annihilation is enhanced at Mg sites (and reduced at Cd sites). An analogous analysis made for the second case (Mg atomic volume) leads to the same conclusion even if there are small differences in the size of effect.

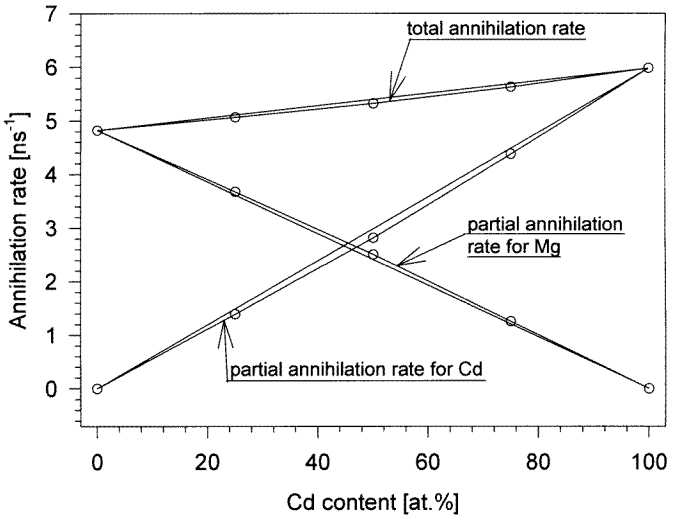

Figure 2. Calculated total and partial positron annihilation rates for the Mg–Cd system. The atomic volume was fixed at the Cd value. The TB–LMTO–GGA scheme (open circles with solid line) was used. See the text for an explanation of straight lines.

The presented results of calculations of the annihilation rate prove that the PPA effect (at Mg sites) is very small for the Mg–Cd system. The PPA at Mg sites is somewhat unexpected because the calculations indicate the charge transfer of 0.1 electron from Mg to Cd and Cd atoms should thereby be more attractive for positrons than Mg ones. Similar calculations performed in the Fe–Al system pointed out a small PPA at Fe sites [8]. In this

system electrons are transferred from Al to Fe atoms and, simultaneously, Fe atoms are preferred by positrons. This is opposite to the Mg–Cd case.

For an experimental confirmation of the PPA one can use the measurement of the DB spectra, where the observation of positron annihilation with core electrons is possible. Our results of the Doppler broadening measurements for pure Mg and Cd are shown in figures 3 and 4. To allow for a comparison between experiment and theory, we calculated the core electron contribution to the DB spectra neglecting the valency electron contribution. We used an approach [20] based on that developed by Alatalo *et al* [11]. The calculations were performed using the TB–LMTO method within the GGA scheme. Usually it is accepted that the core electron contribution to DB spectra dominates for Doppler shifts $|\Delta E| > 4$ keV [11]. A comparison of our experimental and calculated DB spectra is therefore meaningful for energies $E > 515$ keV. Keeping this in mind, we can observe an excellent coincidence of the calculated and measured DB spectra for Mg shown in figure 3. In the case of Cd (figure 4) reasonable agreement with the experimental result was obtained when only seven d electrons on Cd were taken into account in the core contribution. Nevertheless, for energies above 516 keV (∼20 mrad) a small disagreement between theoretical and experimental results is observed, which may be due to the inadequate theoretical description of positron annihilation in a system with d electrons [11].

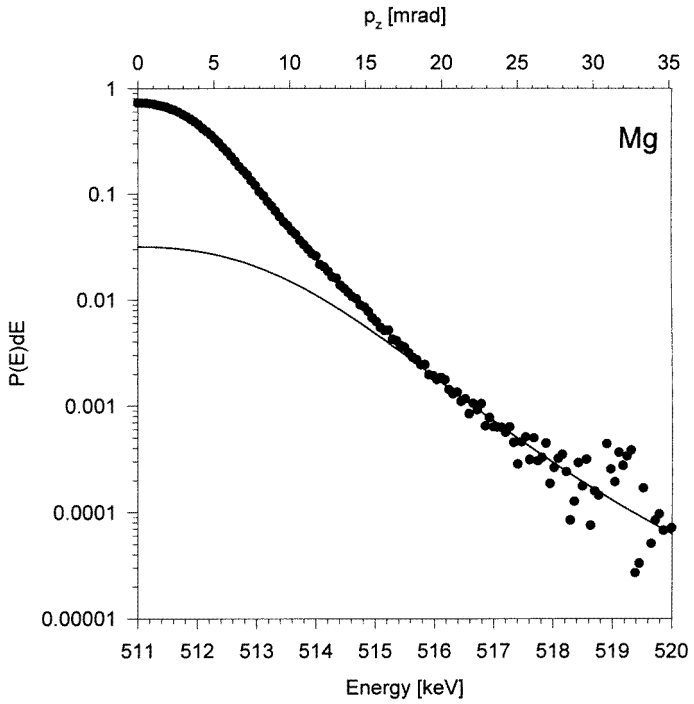

Figure 3. The Doppler broadening spectrum for Mg. The solid line is a result of the TB–LMTO–GGA calculation. On the top axis we use momentum (in mrad units) to characterize the Doppler shift.

Figure 5 presents the values of the W parameter extracted from the DB spectra. The W parameter is defined as a sum of counts per channel in the energy region 514.5–517 keV normalized to the total number of counts in the energy region 511–520 keV. The above

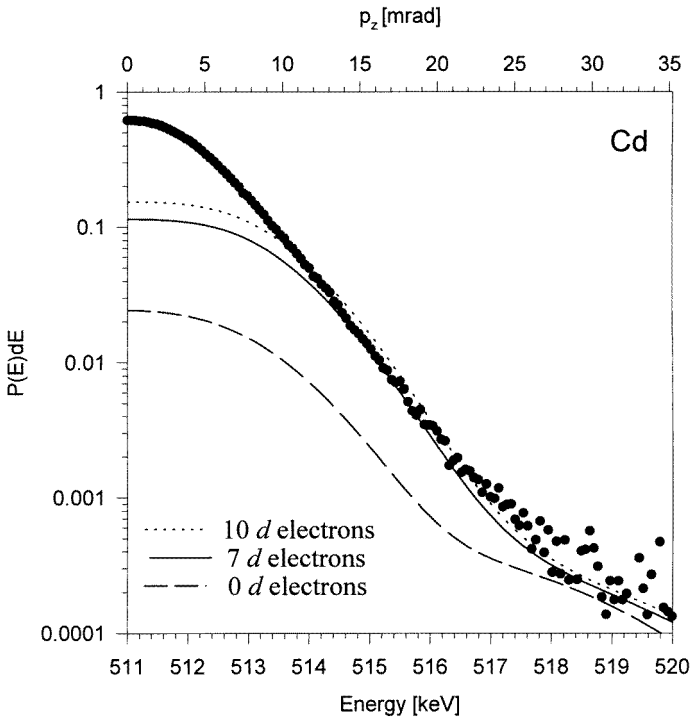

Figure 4. The Doppler broadening spectrum for Cd. The dashed, solid and dotted lines are, respectively, the results of the TB–LMTO–GGA calculations with no, seven and ten d electrons on Cd.

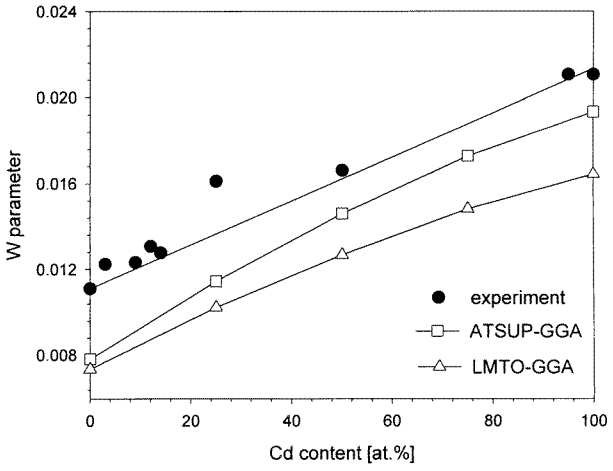

Figure 5. The dependence of the experimental and theoretical values of the *W* parameter on the Cd content. The solid straight line connects the values of the *W* parameter for pure Mg and Cd metals.

defined parameter is sensitive to the positron annihilation with core electrons. We also extracted the same parameter from the calculated DB spectra for Mg–Cd alloys using the

ATSUP and TB–LMTO methods. We can state a good coincidence between the theory and experiment. It should be noticed, however, that the theoretical values are lower than the experimental ones. This is due the fact that the annihilation with valence electrons contributes to the W parameter in the experimental spectra which was neglected in our theoretical calculations. Nevertheless, as in the case of annihilation rate, the ATSUP–GGA scheme gives values closer to the experimental ones. In addition to the W parameter we calculated the core annihilation rate. The procedure of the evaluation of the partial core annihilation rates was the same as described above. We can conclude that the core PPA occurs as well at Mg sites.

As we discussed above, the total positron annihilation rate in an Mg–Cd alloy in an ideal case when no PPA takes place and there are no volume effects would be given by the expression $\lambda(x) = (1 - x)\lambda_{Mg} + x\lambda_{Cd}$. A similar relation would be valid for the DB spectra:

$$\lambda(x)\rho(x) = (1 - x)\lambda_{Mg}\rho_{Mg} + x\lambda_{Cd}\rho_{Cd} \tag{2}$$

where $\rho(x)$, ρ_{Mg} and ρ_{Cd} represent the DB spectra of the alloy with Cd content x, pure Mg and Cd, respectively. The DB spectra are supposed to be normalized to unity. To study the PPA on the basis of the DB measurements, we have to multiply each DB spectrum by the corresponding measured annihilation rate. Figure 6 shows such spectra for Cd, Mg–12.5 at.% Cd and Mg–50 at.% Cd alloys divided by the spectrum of Mg. It is noteworthy that spectra for Mg–12.5 at.% Cd and Mg–50 at.% Cd alloys can be obtained as a simple weighted sum of Mg and Cd spectra. The best coincidence with the measured spectra of these alloys was obtained when the contributions of the Cd spectrum (open circles) were

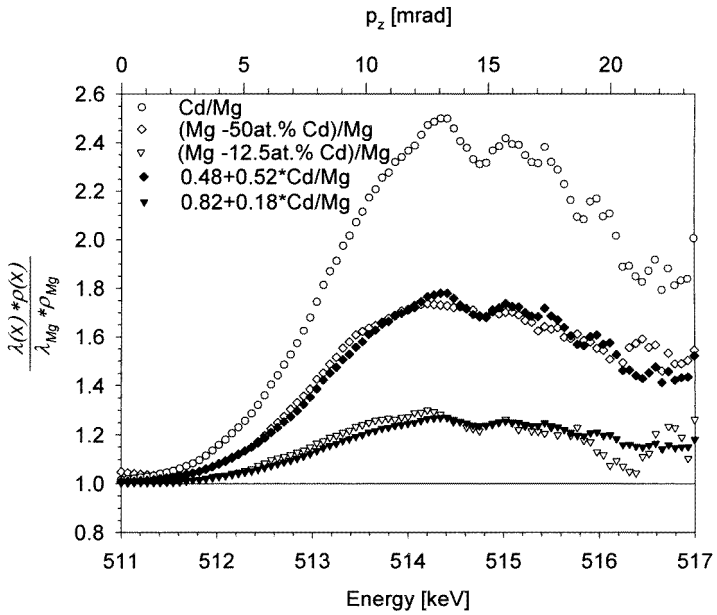

Figure 6. Doppler broadening spectra multiplied by the positron annihilation rate for Cd (open circles), Mg–12.5 at.% Cd (open triangles) and Mg–50 at.% Cd (open squares) samples divided by the analogous spectrum of Mg. The closed triangles correspond to the artificial spectrum obtained as the weighted sum of the Cd spectrum (18%) and Mg spectrum (82%). The closed squares represent also the weighted sum of Cd (52%) and Mg (48%) spectra.

18% and 52%, respectively. This means that the contribution of positron annihilation with Mg (core) electrons is greater in the alloy than in the ideal case (assuming the same Cd content). This further supports arguments for PPA with Mg electrons in the Mg–Cd alloys revealed by the theoretical calculations discussed above. We should mention, however, that we completely neglected the volume effects in our considerations concerning the DB spectra.

3.2. The temperature measurements

The application of positron annihilation spectroscopy to defect studies in metals and alloys has been well described. The energies of vacancy formation were established for number of metals and alloys using the positron trapping model for the description of temperature dependence of the Doppler S parameter, positron lifetime or peak counting rate of the angular correlation curve of annihilation quanta (PCAC). Those temperature dependences may also provide information about the structure changes of the sample. In the Mg–Cd system such changes take place for three ordered solid state phases. For example the α''' phase exhibits peritectoidal decomposition at 186 °C. The order–disorder transformation α''' to α like the other two transformations α' to α and α'' to α is of the first order.

The temperature dependency of the PCAC for pure Cd and Mg–95 at.% Cd samples normalized by the lowest temperature data of each sample is shown in figure 7. These experimental dependences have a conventional form characteristic for positron trapping in thermally generated vacancies in metals. The two-state trapping model was applied to determine the monovacancy formation energy E_W^F. The value (0.49 ± 0.02) eV obtained for Cd is in good coincidence with values given in other papers ([22] and references therein). The value of $E_{1V}^F = (0.35 \pm 0.2)$ eV obtained for Mg–95 at.% Cd has a large uncertainty as the temperature range of the corresponding measurement was limited from room temperature to about 300 °C. The addition of Mg lowers E_{1V}^F as already found in [21].

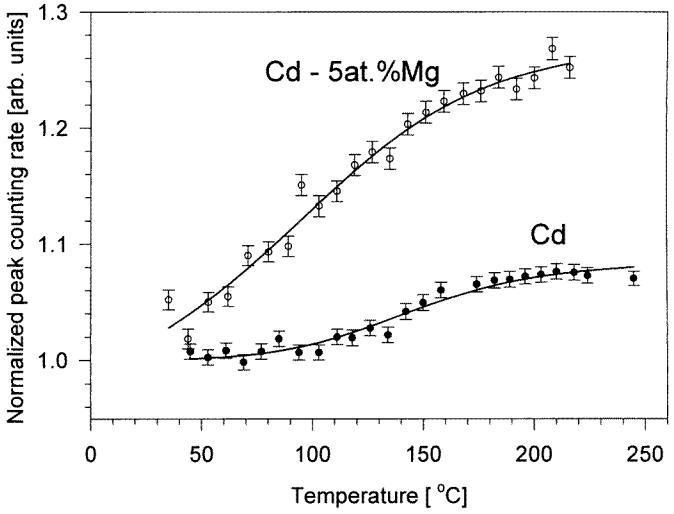

Figure 7. The temperature dependency of the normalized peak counting rate of angular correlation curve for Cd (closed circles) and Mg–95 at.% Cd alloy (open circles). The solid lines present the best fits of the two-state trapping model.

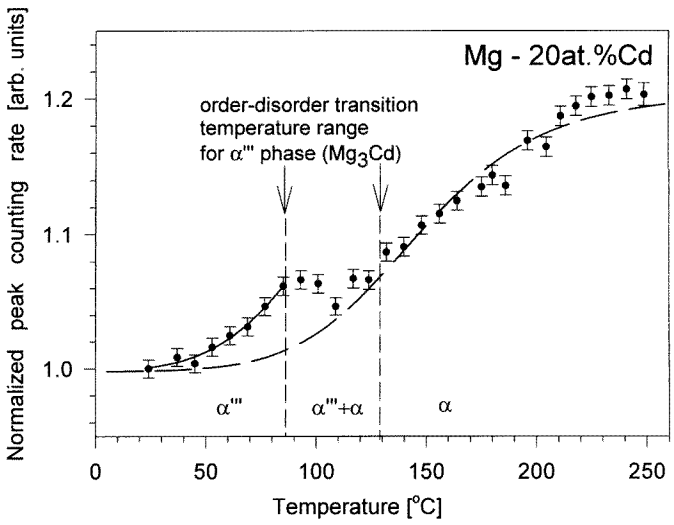

Figure 8. The temperature dependency of the normalized peak counting rate of angular correlation curve for Mg–20 at.% Cd alloy. The solid and the dashed lines present the best fits of the two-state trapping model for ordered and disordered phase regions, respectively.

As far as the alloy Mg–20 at.% Cd is concerned (see figure 8), the increase of temperature causes the increase of the PCAC up to about 80 °C, then the values of the PCAC remain nearly constant up to about 130 °C. Above that temperature the PCAC starts to grow up again. The alloy Mg–20 at.% Cd undergoes a transition from the ordered state which has the hexagonal structure DO_{19} to the disordered A_3 hexagonal structure. Hence, some discontinuity in the increase of the PCAC may be expected. Moreover its temperature range, which extends over 40 °C, matches well with the temperature range of order–disorder transition obtained by, e.g., x-ray diffraction methods [21]. The increase of the PCAC in the region of the ordered alloy was attributed to the creation of thermal vacancies. But in the transition region the thermal energy is used only for the creation of the new disordered phase. Above this temperature region the creation of thermal vacancies continues. The solid and dashed lines in figure 8 denote the results of the best fits of the two-state trapping model in the regions of ordered and disordered phases, respectively. The activation energies of vacancy creation follow from the fitting procedure.

The energy for the disordered alloy is equal to (0.53 ± 0.05) eV and the analogous energy obtained for the part of experimental points corresponding to the ordered alloy is equal to (0.46 ± 0.05) eV. There arises a question of whether that value may be interpreted as the vacancy formation energy for the ordered phase. It seems that the vacancy formation energy for the ordered alloy should be greater than for the disordered alloy. Such a relation is valid at least in the case of the self-diffusion activation energy which is the sum of the vacancy creation energy and the vacancy migration energy (for the vacancy diffusion mechanism). On the other hand, the deviation from stoichiometry for Mg–20 at.% Cd is quite big so that the degree of long-range order is not so high as in the stoichiometric alloy Mg_3Cd. However, differences in crystallographic structures of the ordered and disordered phase may also be responsible for the unexpected relation between the vacancy creation energies.

4. Conclusions

We measured the bulk positron lifetimes in Mg, Cd and selected phases of the Mg–Cd system. The comparison of experimental and theoretical values of the lifetime shows a reasonable coincidence between theory and experiment. Surprisingly, a better agreement with experiment was achieved in the case when the ATSUP approach was used in comparison with the self-consistent TB–LMTO technique.

We found that the dependence of the bulk positron annihilation rate on the Cd content is nonlinear, but it is well described by the empirical formula proposed by Seeger and Banhart [19] which relates the annihilation rate and atomic volume. The PPA in the Mg–Cd system is thus hardly detectable when just positron lifetime (annihilation rate) is measured. However, the concentration dependences of the Mg and Cd partial annihilation rates calculated using the TB–LMTO method at a constant atomic volume indicate a small PPA with Mg electrons. The analysis of the core annihilation rates leads to the same conclusion. The PPA at Mg sites is further confirmed by the comparison of the DB spectra for Mg–12.5 at.% and Mg–50 at.% Cd samples with a linear combination of the Mg and Cd spectra.

We also studied the temperature dependences of the peak counting rate of the angular correlation curve. The application of the two-state trapping model allowed for the determination of the monovacancy formation energy for Cd and Mg–95 at.% Cd samples. We can state that the addition of Mg to Cd leads to a decrease of the monovacancy formation energy. In the case of the Mg–20 at.% Cd alloy the order–disorder phase transition was observed and the vacancy formation energies for the ordered and disordered phase were established.

Acknowledgments

Thanks are due to O K Andersen and O Jepsen for providing their TB–LMTO–ASA code. We also thank M Puska and T Korhonen for permitting us to use their LMTO positron and ATSUP codes. One of the authors (ED) acknowledges financial support from the Committee of Scientific Research (Poland) for supporting this work under grant No 175 PO3 97 13.

References

[1] Stott M J and Kubica P 1975 *Phys. Rev.* B **11** 1
[2] Kubica P, McKee B T A, Stewart A T and Stott M J 1975 *Phys. Rev.* B **11** 11
[3] Szotek Z, Gyorffy B L, Stocks G M and Temmerman W M 1984 *J. Phys. F: Met. Phys.* **14** 2571
[4] Dębowska E and Rudzińska-Girulska J 1988 *Phys. Scr.* **39** 767
[5] Wegner D and Lühr-Tanck W 1987 *J. Phys. F: Met. Phys.* **17** L289
[6] Balogh Á G, Bottyán L, Brauer G, Dési I and Molnár B 1986 *J. Phys. F: Met. Phys.* **16** 1725
[7] Dębowska E 1992 *Acta Universitatis Wratislaviensis* 1419
[8] Kuriplach J, Šob M and Dauwe C 1997 *Nukleonika* **42** 153
[9] Moser Z, Gąsior W, Wypartowicz J and Zabdyr L 1984 *Bull. Alloy Phase Diagrams* **5** 23
[10] Raynor G V 1959 *The Physical Metallurgy of Magnesium and its Alloys* (New York: Pergamon)
[11] Alatalo M, Barbiellini B, Hakala M, Kauppinen H, Korhonen T, Puska M J, Saarinen K, Hautojärvi P and Nieminen R M 1996 *Phys. Rev.* B **54** 2397
[12] Puska M J and Nieminen R M 1983 *J. Phys. F: Met. Phys.* **13** 333
[13] Anderson O K, Jepsen O and Šob M 1987 *Electronic Structure and its Application* ed M Yussouff (Heidelberg: Springer) p 1
[14] Kansy J 1996 *Nucl. Instrum. Methods* A **374** 235
[15] Dryzek J and Dryzek E 1997 *Nukleonika* **42** 87
[16] Barbiellini B, Puska M J, Korhonen T, Harju A, Torsti T and Nieminen R M 1996 *Phys. Rev.* B **53** 16 201
[17] Djourelov N and Misheva M 1996 *J. Phys.: Condens. Matter* **8** 2081

[18] Boroński E and Nieminen R M 1986 *Phys. Rev.* B **34** 3820
[19] Seeger A and Banhart F 1987 *Phys. Status Solidi* **102** 171
[20] Kuriplach J, Van Hoecke T, Van Waeyenberge B, Dauwe C, Segers D, Balcaen N, Morales A L, Trauwaert M-A, Vanhellemont J and Šob M 1997 *Mater. Sci. Forum* **225–227** 605
[21] Belaidi A, Leighly H P, Coleman P G and West R N 1987 *Phys. Status Solidi* **102** 127
[22] Frantz C and Gantois M 1971 *J. Appl. Crystallogr.* **4** 387