ON THE POSITRON ANNIHILATION PROCESS IN $\text{Ni}_{1-c}\text{Cu}_c$ ALLOYS.*

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We present new, accurate, calculations of the electron momentum distribution function for the $\text{Cu}_{1-c}\text{Ni}_c$ random solid solution and discuss, in quantitative terms, the role played by the positron wavefunction in determining the Angular Correlation of the Annihilation Radiation (ACAR).

1. INTRODUCTION

One of the most interesting prediction of the Korringa-Kohn-Rostoker-Coherent Potential Approximation (KKR-CPA) calculations of the electronic structure in random substitutional metallic alloys is that these systems possess well defined Fermi Surfaces at all concentrations [1]. This is a consequence of the fact that the Bloch spectral function, $A(\vec{k};\epsilon)$ consists of peaks well defined in energy on the scale of the separation between bands and localized in $\vec{k}$ -space with widths $\delta k \ll 'k'$, the linear dimension of the Fermi Surface. This suggests that the ground-state and response properties of the electron liquid in these alloys will be as dominated by the (slightly smeared) Fermi Surface as in the case of pure metals. For instance, it has been shown, recently, that parallel, flat sheets of the Fermi Surface can drive concentration waves, ordering processes, with periodicity determined by the spanning vector in such alloys as CuPd_{1-c} [2]. This phenomenon is a replacement analogue of the displacive Periodic Lattice Distortions (PLD or CDW) in ordered metals such as NbSe_2 , TaSe_2 etc.

Evidently, under these circumstances a systematic exploration of the geometrical and other properties of Fermi Surfaces in random metallic alloys is an urgent and interesting task.

The most suitable experimental technique for this purpose is the 2-d measurement of ACAR [3]. In order to facilitate the interpretation of these, a number of first principles (KKR-CPA) calculations of the configurationally averaged electron momentum distribution, $\bar{\rho}(\vec{p})$, have been performed for CuNi_{1-c} [4] and AgPd_{1-c} [5] alloys. Here we report a new calculation of $\bar{\rho}(\vec{p})$, in the L -direction, for $\text{Cu}_{1-c}\text{Ni}_c$. It is based on the most reliable potential function, which has been recently tested in an Angleresolved-Photoemission experiment. [6]. We have also solved the KKR-CPA equations for the positron and present a preliminary study of the positron wave function in this and other alloys.

2. THE ELECTRON MOMENTUM DISTRIBUTION

 $\bar{\rho}(\vec{p})$ IN $\text{Cu}_{1-c}\text{Ni}_c$

In the language of multiple scattering theory on the energy shell [1,7].

$$\bar{\rho}(\vec{p}) = -\frac{1}{\pi\Omega_0} \text{Im} \sum_{\alpha,L,L'} \left\{ \sum_{\alpha,L,L'} C_{\alpha} \Delta_L^{\alpha}(\vec{p},\epsilon) \Delta_{L'}^{\alpha}(-\vec{p},\epsilon) \langle \tau_{LL'}^{\alpha}(\epsilon) \rangle_{n\alpha} \right\} + \frac{1}{n} \sum_{n\alpha} \sum_{\alpha,L,L'} e^{i\vec{p}(\vec{R}_n - \vec{R}_{L'})} \Delta_L^{\alpha}(\vec{p},\epsilon) \Delta_{L'}^{\alpha}(-\vec{p},\epsilon) \langle \tau_{LL'}^{\alpha}(\epsilon) \rangle_{n\alpha}, \quad (1)$$

where Ω_0 is the volume of a unit cell, L stands for the angular momentum quantum numbers l, m , $\alpha \equiv \text{Cu or Ni}$, C_{α} is the concentration of the α -type atoms, $\langle \rangle_{n\alpha}$ and $\langle \rangle_{n\alpha;m,l}$ denote partial averages such that $\langle \rangle_{n\alpha}$ there is an α -type atom at the n -th site whose position vector is $\vec{R}$ and a β atom at $\vec{R}_{L'}$, $\tau_{LL'}^{\alpha}(\epsilon)$ is the real space KKR-matrix $t_{LL'}^{\alpha}(\epsilon)$ for a given configuration and $\Delta_L^{\alpha}(\vec{p};\epsilon)$ is the L -th component of the momentum space scattered wave due to a single α -type potential well. In terms of the L the partial wave component of the 'on the energy shell' t -matrix describing the scattering of an electron at the n -th site, $t_{LL'}^{\alpha}(\epsilon)$, $\tau_{LL'}^{\alpha}(\epsilon)$ may be written as

$$\tau_{LL'}^{\alpha}(\epsilon) = [t_{LL'}^{\alpha}(\epsilon) \delta_{nn} - G_{LL'}(\vec{R}_n - \vec{R}_{L'},\epsilon)]^{-1},$$

where $G_{LL'}(\vec{R}_n - \vec{R}_{L'},\epsilon)$'s are the real space structure constants. Also

$$\Delta_L^{\alpha}(\vec{p},\epsilon) = 4\pi \sum_{l'} i^{l'} Y_{l'}(\vec{p}) \int d^3r R_L^{\alpha}(r,\epsilon) j_{l'}(pr) Y_{l'}(\vec{r}) Y_{l'}(\vec{r}), \quad (2)$$

where $R_L^{\alpha}(r,\epsilon)$ is a radial solution for an α -type well normalized to match smoothly to a scattered wave, the $j_{l'}(pr)$'s are Bessel functions and the $Y_{l'}^m$'s are real spherical harmonics.

Within the framework of the KKR-CPA there is a well defined expression for the partial average $\langle \tau_{LL'}^{\alpha}(\epsilon) \rangle_{n\alpha}$ [7]. Using this in Eq. 1 leads to the formula discussed in ref. 6. The results of our calculations based on this is shown in Fig. 1.

As expected the dominant feature of $\bar{\rho}(0,0,p_z)$ is a sharp drop at the 'radius' of the Γ -centred sheet of the Fermi Surface. An interesting alloying feature is the rise before this fall. This is due to the fact that the s -band, having emerged from the Ni 'impurity'

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Figure 1: The electron momentum density $\bar{\rho}(\vec{p})$ in $\text{Cu}_{60}\text{Ni}_{40}$ alloy. Curve 1 gives $\bar{\rho}(\vec{p})$ along $\vec{p} = (0, 0, p_z)$ for $0 < p_z < 2$. Curve 2 gives $\bar{\rho}(\vec{p})$ along $\vec{p} = (1, 1, 1+p_z)$ for $0 < p_z < 1$.

band, sharpens up faster than it rises towards ϵ_F . This is probably a quite general behaviour in alloys and has nothing to do with electron-positron correlations which is well known to give rise to similar behaviour.

3. THE 2γ -RAY MOMENTUM DISTRIBUTION FUNCTION $\bar{\rho}_{2\gamma}(\vec{p})$

Within the above formalism it is straightforward to calculate $\bar{\rho}_{2\gamma}(\vec{p})$ which depends not only on the electron momentum distribution but also on the positron wave function. One finds that

$$\bar{\rho}_{2\gamma}(\vec{p}) = \sum_{l_1 l_2 l_3} \int_{-\infty}^{\epsilon_F} \frac{d\epsilon}{\pi} \int_{-\infty}^{\epsilon_F} \frac{d\epsilon'}{\pi} \left\{ \sum_{\alpha} C_{\alpha} \Delta_{l_1 l_2}^{\alpha}(\vec{p}, \epsilon, \epsilon') + \sum_{m \neq n} \sum_{\alpha \beta} C_{\alpha} C_{\beta} \Delta_{l_1 l_2}^{\alpha}(\vec{p}, \epsilon, \epsilon') \Delta_{l_3 l_2}^{\beta}(-\vec{p}, \epsilon, \epsilon') + \sum_{m \neq n} \sum_{\alpha \beta} \langle \mathcal{J}_m \tau_{l_1 l_2}^{e, nm}(\epsilon) \mathcal{J}_n \tau_{l_3 l_2}^{p, mn}(\epsilon') \rangle_{n \alpha m \beta} \right\}, \quad (3)$$

where $\tau_{l_1 l_2}^{e, nm}(\epsilon)$ is the same as $\tau_{l_1 l_2}^{nm}(\epsilon)$ in Eq. 1, $\tau_{l_3 l_2}^{p, mn}(\epsilon')$ is the analogous quantity for the positron and the new matrix elements $\Delta_{l_1 l_2}^{\alpha}(\vec{p}; \epsilon, \epsilon')$ involve both electron and positron $l_1 l_2$ wave functions. The most significant component is given by

$$\Delta_{0,0}^{\alpha}(\vec{p}, \epsilon, \epsilon') \propto \int_0^{2\pi} d\phi r^2 R_{l=0}^{e, \alpha}(r, \epsilon) R_{l=0}^{p, \alpha}(r, \epsilon') j_{l=0}(pr), \quad (4)$$

where $R_{l=0}^{e, \alpha}$ and $R_{l=0}^{p, \alpha}$ are radial solutions for a positron and an electron respectively at an u -type of site (the positron 'sees' a potential which is the negative of that 'seen' by an electron corrected for the absence of exchange interaction).

Again the CPA makes a very specific prediction for the partial averages which takes into account the vertex corrections. However, the most relevant vertex corrections are already included in the simple approximation:

$$\langle \tau_{l_1 l_2}^{e, nm}(\epsilon) \tau_{l_3 l_4}^{p, mn}(\epsilon') \rangle_{n \alpha m \beta} = \langle \tau_{l_1 l_2}^{e, nm}(\epsilon) \rangle_{n \alpha} \langle \tau_{l_3 l_4}^{p, mn}(\epsilon') \rangle_{m \beta}$$

This decoupling takes proper account of the concentration fluctuations at the sites where the e-p annihilation takes place. Further corrections are likely to be small for many alloys where the scattering of positrons at different type of sites are very similar. As we shall now show this will be the case surprisingly often.

In order to investigate the behaviour of positrons in random alloys we have constructed positron potentials (Mattheiss prescription without exchange contribution) for a number of systems. The scattering phase shifts for the first two partial waves in a selection of cases are shown in Figure 2.

Figure 2: Comparison of s, p and d positron phase shifts for Cu, Ni, Mo, Nb and Pt in $\text{Cu}_{60}\text{Ni}_{40}$, $\text{Mo}_{50}\text{Nb}_{50}$ and $\text{Pt}_{50}\text{Ni}_{50}$ alloys, respectively. (a) shows Cu and Ni phase shifts in $\text{Cu}_{60}\text{Ni}_{40}$; (b) gives Mo and Nb phase shifts in $\text{Mo}_{50}\text{Nb}_{50}$; (c) represents Pt and Ni phase shifts in $\text{Pt}_{50}\text{Ni}_{50}$.

The corresponding pure metal positron band-structures are shown in Figure 3.

Figure 3: The positron energy band structure along ΓX and ΓL directions for Cu, Ni and Pt in $\text{Cu}_{60}\text{Ni}_{40}$ and $\text{Pt}_{50}\text{Ni}_{50}$ alloys. The results for positron energy band structure along ΓH and ΓP directions for Mo and Nb in $\text{Mo}_{50}\text{Nb}_{50}$ alloy are also plotted for comparison. They are based on the muffin-tin potentials of the respective constituents of these alloys.

Evidently the positron hardly sees the difference between the different type of sites in $\text{Cu}_{60}\text{Ni}_{40}$ and $\text{Nb}_{50}\text{Mo}_{50}$, but a Ni site is significantly less repulsive than a Pt site in $\text{Ni}_{50}\text{Pt}_{50}$.

In Figure 4 we show the KKR-CPA Bloch spectral functions for the electrons, $\tilde{A}_B^e(k, \epsilon)$, and the positrons, $\tilde{A}_B^p(k, \epsilon)$, respectively at the Γ -point in the case of $\text{Cu}_{60}\text{Ni}_{40}$. This figure depicts the bottom of the positron s-band relative to the electronic states.

We have evaluated $\Delta_{0,0}^a(\vec{p}, \epsilon, \epsilon')$ and found that its shape does not differ much from its electron only counterpart. Clearly, in this alloy we may expect that $\tilde{p}_{2\gamma}(\vec{p})$ will be a slightly smeared version of $\tilde{p}(\vec{p})$. Further calculations are in progress and will be published elsewhere.

We conclude that for many alloy systems the positron spectra is not very sensitive to substitutional disorder and the simple decoupling scheme proposed in Eq. 3 should provide an adequate basis for calculating $\tilde{p}_{2\gamma}(\vec{p})$.

Figure 4: Electron and positron Bloch spectral functions for Γ -point in $\text{Cu}_{60}\text{Ni}_{40}$ alloy. Positron Bloch spectral function occurs as a vertical line at the bottom of Cu-d band in this particular alloy.

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