phys. stat. sol. (b) **210**, 177 (1998)

Subject classification: 71.20.Be; 71.15.Ap; 72.15.Jf; S1; S1.2; S1.3

Calculation of Electronic Structure and Diffusion Thermopower of Cu–Ni and Ag–Pd Alloys by the APW-VCA Method

A. S. Karolik and V. M. Golub

Institute of Applied Physics, National Academy of Sciences of Belarus, Minsk

(Received July 23, 1998)

Schoen's augmented-plane-wave virtual-crystal approximation (APW-VCA) is used first for calculation of the density of electronic states and electronic properties of disordered substitutional metal alloys. The electronic specific heat coefficient and the diffusion thermopower of Ag_xPd_{1-x} and Cu_xNi_{1-x} alloys as a function of concentration are calculated. The calculation used no adjustable parameters. The results are compared with experiment and with previous calculations performed in the framework of CPA. It is shown that the agreement with experiment is not worse than within CPA, and at a low concentration of the noble metal it is even better.

Приближение виртуального кристалла Шоена на базе метода присоединенных плоских волн (ППВ-ПВК) использовано впервые для расчета плотности электронных состояний и электронных свойств неупорядоченных металлических сплавов замещения. Рассчитаны коэффициент электронной удельной теплоемкости и диффузионная термо ЭДС сплавов Ag_xPd_{1-x} и Cu_xNi_{1-x} как функция концентрации. Расчет не содержит подгоночного параметра. Результаты расчета сравниваются с экспериментом и расчетами, выполненными в ПКП. Показано, что согласие с экспериментом получено не хуже, чем с использованием ПКП, а при низкой концентрации благородного металла, даже лучше.

1. Introduction

Among a variety of theoretical models of alloys, used for calculation of the electronic structure and properties of disordered alloys, the most wide employment has found the coherent potential approximation (CPA) [1 to 4]. At present the CPA is considerably improved and developed on the base of various methods of band calculations (TB, KKR, LMTO, LCAO and others) [1 to 10]. Within the framework of this approach rather significant success in calculations of the electronic density of states, optical properties and parameters of the Fermi surface of substitutional alloys, first of all transition metals with noble metals, has been achieved. However, the first-principles calculations within CPA of electronic properties such as the electronic specific heat, conductivity and thermoelectric power do not always show good quantitative agreement with experiment, particularly for alloys with a high concentration of the transition metal component. Moreover, the results of the CPA calculations show a strong dependence on the splitting parameter, determining the energy interval between d-resonances of the alloy components [1 to 3, 6, 7], the choice of which affects largely the energy-band shape near the Fermi energy.

Here we report the results of calculation of the electronic structure and some properties of disordered transition–noble metal alloys performed by the augmented-plane-wave method on the base of Shoen's virtual-crystal approximation (VCA) [11]. In contrast to the better known virtual-crystal model (VCM) [12], using the average potential of components weighted by their fractional atomic concentrations and a result giving a single set of averaged bands, the VCA allows to build a multicomponent alloy MT-potential, which is treated correctly in the perfect-crystal technique. As a result we obtain the band set for each component and can disclose the individual features of the electronic structure of the constituents. Another distinction is that the VCM describes adequately the electronic structure of an alloy only when the constituent energy bands are rather similar, rather wide and if band centre separation is small. The APW-VCA has not such limitations. Unfortunately, the APW-VCA is an non-self-consistent procedure. As it has been noted in [13], that the errors in the assumed average potential between the MT-spheres may lead to incorrect spacings between the energy bands, but that does not change significantly their shapes. That is why the transport properties, which are defined by the energy-band shape at the Fermi surface are rather well described by this method.

The APW-VCA was developed by Shoen [11] for disordered solid solutions and non-stoichiometric compounds and had been used successfully for the calculation of non-stoichiometric compounds. As has been shown in [13], a quite satisfactory agreement with experiment in calculations of the resistivity, absolute thermoelectric power and Hall coefficient for TiO in the frame work of the APW-VCA has been obtained. However, as we know, for metalic solid solutions the APW-VCA method was not used.

We present the results of calculation of the electronic density of states, the electronic specific heat and the absolute diffusion thermopower of disordered Cu–Ni and Ag–Pd alloys for the whole range of concentrations. In this paper we regard paramagnetic substitutional solid solutions. A special attention is given to the analysis and calculation of the diffusion thermoelectric power. The thermopower is more difficult for a theoretical description than, for example, conductivity. So at present the influence only of small additions of impurities (<1 at%) on the thermopower of alloys is calculated successfully, when Matthiessen's rule is valid and the Fermi surface of the host metal does not vary essentially [15, 16]. Usually such works are connected with the calculation of the characteristic thermopowers of impurities. The thermoelectric properties of more concentrated solid solutions are usually described either qualitatively [17, 18], or quantitatively but with using fitting or connected with experiment parameters [19, 20]. The first-principles calculations, as a rule, poorly correlate with experiment [21, 5]. The most significant progress in this problem has been achieved for Ag_xPd_{1-x} alloys in the framework of KKR-CPA for the range of values x from 0.2 up to 0.8 [5].

The choice of the Cu–Ni and Ag–Pd alloys as objects for our calculations is defined by the fact that these alloys are investigated experimentally more completely. These alloys form random solid solutions over the entire concentration range with the same crystal structure. The lattice parameters differ only by some percentages. They are convenient objects for the application of the APW-VCA method. Because charge transfer effects in these alloys are unimportant [8, 10] it is possible to build the MT-potentials for the pure metal components quite exactly and then to perform their linear interpolation within the intermediate range. Furthermore, Ag–Pd is the only alloy, for which the first-principles calculations of thermopower as functions of concentration over a wide range of its changes have been successfully performed. Therefore, the comparison of results obtained by different methods is of interest.

2. Thermopower of the Transition – Noble Metal Alloys

One of the earliest models, used for the explanation of thermoelectric properties of alloys of transition metals with noble ones was the "rigid band" approach [22, 23]. The model described satisfactorily (mostly qualitatively) the behaviour of the thermopower only for transition-metal-rich alloys, when the perturbation, created by a monovalent impurity in the electronic structure of the host metal, was negligible. For noble-metal-rich alloys this model did not give even a qualitative interpretation. It is connected with a strong disturbance of the electronic energy structure of the noble-metal solvent by transition-metal impurities. That results in the formation of an additional d-subband near the Fermi energy of the alloys. The height and width of the additional d-peak increases with the concentration of the transition-metal constituent.

The thermopower is a property, very sensitive to tiny changes of the electronic structure near the Fermi energy of the metal. An addition of less than 1 at% of the transition-metal impurity (for example Ni or Pd) in a noble-metal solvent causes a substantial change of the absolute thermopower of alloys and even the inversion of sign [24]. It is the evidence of the qualitative change of scattering mechanism of s-electrons, which begin to scatter by vacant states of the d-subband. Thus, for such alloys Mott's theory may be already applied, starting from a small concentration of transition impurities [22].

We assume, that the density of electronic states at the Fermi energy E_F in the d-band N_d is much larger than its value in the s-band N_s, already, beginning from several atomic percents of the transition-metal impurity. As a result the effective mass $m_d^* > m_s^*$, and conductivity $\sigma_s > \sigma_d$, so that for the absolute thermopower of a double-band conductor

$$S = \frac{\sigma_s S_s + \sigma_d S_d}{\sigma_s + \sigma_d} . \tag{1}$$

As first approximation the following expression [15] will be valid

$$S = S_s = -\frac{\pi^2 k_B^2 T}{3|e|} \left(\frac{\mathrm{d} \ln \sigma_s}{\mathrm{d}E} \right)_{E=E_F} , \tag{2}$$

where S_s, S_d and σ_s, σ_d are the absolute thermopowers and electric conductivities in s- and d-bands, respectively, k_B is the Boltzmann constant. Here

$$\sigma_s(E) \sim \tau_s(E)\, v_s(E)\, F_s(E) ,$$

where v is the velocity of electrons, F the area of the Fermi surface, τ_s the relaxation time of s-electrons, here $\tau_s^{-1} = \tau_{ss}^{-1} + \tau_{sd}^{-1}$. Taking into account that $\tau_{sd}^{-1} \sim N_d$ and $\tau_{ss}^{-1} \sim N_s$, and assuming that the connecting constants are equal, we shall obtain that $\tau_s^{-1} \sim N$, where $N = N_s + N_d$. Then the absolute coefficient of diffusion thermopower is written as

$$S = \frac{\pi^2 k_B^2 T}{3|e|\, E_F} \left[\frac{\mathrm{d} \ln N}{\mathrm{d} \ln E} - \frac{\mathrm{d} \ln (vF)}{\mathrm{d} \ln E} \right]_{E=E_F} . \tag{3}$$

The second term in the square brackets for Cu–Ni and Ag–Pd alloys does not exceed its value in the free electron model, equal to 3/2. So, for copper, for example, it is about 0.4 [25, 26]. The Fermi surfaces of copper, nickel, silver, palladium and their alloys are identical, they are spheres distorted by the necks due to contact with boundaries of the Brillouin zone. Differences occur only in the degree of the contact. In our estimations the contribution of the second term in the absolute thermopower of the considered alloys does not exceed 1 μV/K. The first term in the brackets is much larger and already above 10 at% Ni or Pd it is higher by an order of magnitude. Therefore, for these alloys a quite good approximation for the diffusion thermopower will be the expression

$$S = \frac{\pi^2 k_\mathrm{B}^2 T}{3|e|} \, \frac{1}{N(E_\mathrm{F})} \left(\frac{\mathrm{d}N}{\mathrm{d}E}\right)_{E_\mathrm{F}} . \tag{4}$$

Earlier, on the basis of this expression the qualitative explanation of the concentration dependence of diffusion thermopower and volume piezothermoelectric effect for Cu–Ni alloys has been given [27].

3. Method of Calculation

For calculation of the electronic energy structure of substitutional alloys the augmented-plane-wave virtual-crystal approximation (APW-VCA) was used [11]. As we use the non-self-consistent APW method, the initial approach for the potential was previously checked in calculations of the electronic structure and properties of the pure metal components [14]. It is possible within this approach to construct the average muffin-tin potential for each alloy component. With this aim the self-consistent Roothaan-Hartree-Fock atomic wave-functions were used [28]. Their advantage is the analytical representation convenient for subsequent dealing with alloys. The expansion coefficients for pure metals are defined in [28]. For the alloys considered here we assume that these coefficients are linear functions of concentration.

The average Coulomb potential in the MT-sphere is [11]

$$V_\mathrm{c}(\mathbf{r}) = V_k(\mathbf{r}) + \sum_t n_t \sum_\eta c_{\eta t} V_\eta(R_t, \mathbf{r}) , \tag{5}$$

where $V_k(\mathbf{r})$ is the Coulomb potential of the k-th atom, $V_\eta(R_t, \mathbf{r})$ is the contribution to the Coulomb potential due to the η-th alloy component of neighbouring shells t, R_t is the radius of the t-shell, n_t is the number of atoms in the t-shell, $c_{\eta t}$ is the fractional atomic concentration of the component.

The exchange potential V_x was built in the Slater approximation with the exchange-correlation parameter α,

$$V_\mathrm{x}(\mathbf{r}) = -6\alpha \left\{ \frac{3}{8\pi} \left[\varrho_k(\mathbf{r}) + \sum_t n_t \sum_{\eta=1}^{2} c_{\eta t} \varrho_\eta(R_t, \mathbf{r}) \right] \right\}^{1/3} . \tag{6}$$

Here $\varrho_k(\mathbf{r})$ is the charge density of the k-th atom, $\varrho_\eta(R_t, \mathbf{r})$ is the contribution to the charge density due to atoms of η-th sort of t-shell. The exchange and Coulomb potentials are the average over all equivalent lattice sites. The exchange parameter α for pure metals components was chosen such as to satisfy the virial theorem, that allowed to take into account both the exchange and correlation effects, and is for Cu, Ni, Ag and Pd, 0.70635, 0.70843, 0.70114 and 0.70128, respectively [29]. For the considered alloys the parameter α was believed linear in concentration too.

The constant potential between MT-spheres, V_c, was calculated by averaging of the muffin-tin potential over the area between the radius of MT-sphere and that of Wigner-

Seitz cell. Both these values are functions of the alloy lattice parameters a,

$$a = xa_t + (1 - x)\, a_n\,,$$

where a_t and a_n are the lattice parameters of transition and noble metals, respectively, x is the concentration of the transition component.

The Schrödinger equation has been solved using 27 APW waves. The summation over angular momentum states up to $l = 12$ has been carried out. The matrix elements of the secular equation had the form

$$H_{ij} = (\mathbf{k}_i\mathbf{k}_j - E)\,\delta_{ij} - \sum_{s=1}^{p} \frac{4\pi(R^{s}_{\mathrm{MT}})^2}{\Omega_0}\, \mathrm{e}^{ik_{ij}r_s}\, F_{ij,\mathrm{s}}\,, \tag{7}$$

where

$$\begin{aligned} F_{ij,\mathrm{s}} &= (\mathbf{k}_i\mathbf{k}_j - E)\, j_1(k_{ij}R^{\mathrm{s}}_{\mathrm{MT}})/k_{ij} \\ &\quad - \sum_{l} (2l+1)\, P_l(\cos\theta_{ij})\, j_l(k_iR^{\mathrm{s}}_{\mathrm{MT}})\, j_l(k_jR^{\mathrm{s}}_{\mathrm{MT}}) \sum_{\eta} C_{\eta s} L^{\eta}_{l}(E, R^{\mathrm{s}}_{\mathrm{MT}})\,. \end{aligned}$$

Here $\mathbf{k}_i = \mathbf{k} + \mathbf{K}_i$, $\mathbf{k}_{ij} = \mathbf{K}_i - \mathbf{K}_j$; $\mathbf{K}_i$ is the reciprocal lattice vector, Ω_0 is the volume of the unit cell, $\mathbf{r}_s$ is the vector from the centre of a cell to the s-th site in the cell, $R^{\mathrm{s}}_{\mathrm{MT}}$ is the radius of the s-th MT-sphere, θ_{ij} is the angle between the $(\mathbf{k}+\mathbf{K}_i)$ and $(\mathbf{k}+\mathbf{K}_j)$ reciprocal lattice vectors, L^{η}_{l} is the logarithmic derivative of the l-th radial wave function on the surface of the MT-sphere.

The procedure of integration over the Brillouin zone was carried out by the method of tetrahedra [30]. The number of electrons per atom in the conduction band was assumed equal $n = 11 - x$.

4. Results

In this paper the following atomic electron configurations of pure metals were used: Cu ($3d^{10}4s^1$), Ni ($3d^{9.4}4s^{0.6}$), Ag ($4d^{10}5s^1$), Pd ($4d^9 5s^1$). In view of using the non-self-consistent APW method the initial approach was previously examined in calculations of the electronic energy structure and properties of pure metal components. The good or quite satisfactory accordance with available experimental data and results of earlier self-consistent calculations have been obtained in calculations of the electronic energy structure, some characteristic energy intervals, the Fermi surface paramaters and the specific heat coefficients [14]. The best agreement has been achieved for copper and nickel.

The electron densities of states functions $N(E)$ were calculated for $\mathrm{Ag}_x\mathrm{Pd}_{1-x}$ and $\mathrm{Cu}_x\mathrm{Ni}_{1-x}$ alloys across the complete range of concentration in steps of 0.1 on x. The results of the calculation of the total and partial densities of states are represented in detail in [31, 32] for CuNi and AgPd systems, respectively. In Fig. 1 we represent the results for two concentrations only, $\mathrm{Cu}_{0.8}\mathrm{Ni}_{0.2}$ and $\mathrm{Cu}_{0.2}\mathrm{Ni}_{0.8}$ as illustration. The calculated dependencies $N(E)$ are compared with results of previous calculations carried out within the coherent potential approximation in the frame work of TB [1], KKR [7] and LCAO [10] methods. The available experimental dependencies on the base of ultraviolet photoemission data (UPS) [35] for close concentrations are shown too. All curves have been shifted so that the Fermi energies coincide at the same energy scale. The Fermi energy is indicated by the vertical line. The main features of the density of states

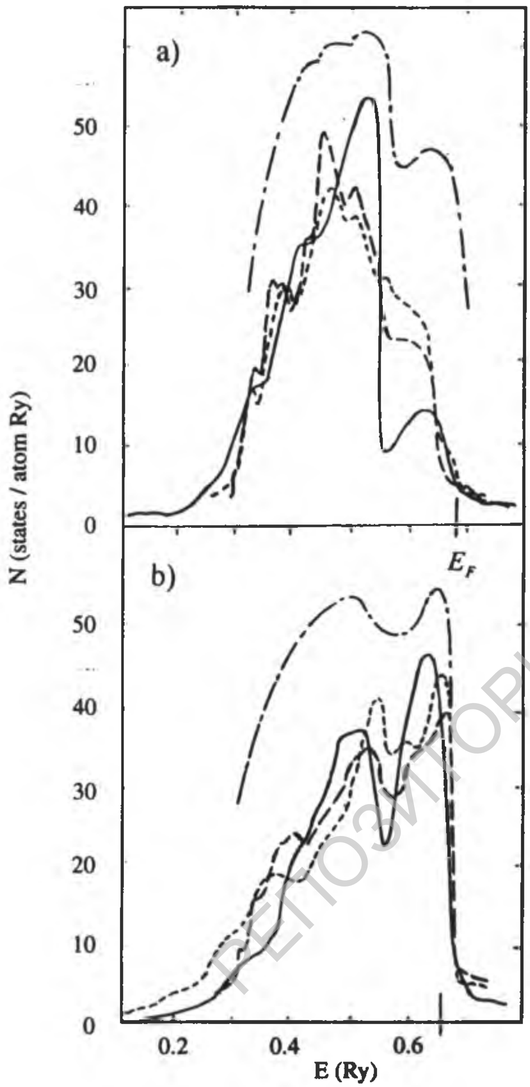

Fig. 1. Comparison of the electronic density of states for the alloys a) $Cu_{0.8}Ni_{0.2}$ and b) $Cu_{0.2}Ni_{0.8}$ calculated by various methods: full line: APW-VCA (present work); dashed line: KKR-CPA [7]; short-dashed line in a): LCAO-CPA [10]; short-dashed line in b): TB-CPA [1]; the dash-dotted lines represent the experiment [35]. All curves are superposed so that the Fermi energies coincide at the same energy scale

functions and the arrangement of d-peaks with respect to the Fermi energy E_F correlate with the experimental data rather well. So according to the photoemission measurements, the additional d-peak in Ag-rich silver–palladium alloys is located in the range of 2.0 to 2.1 eV (or 0.15 Ry) below E_F [33, 34]. In our calculation this energy interval is 0.16 Ry. The two main d-peaks in the $Cu_{0.19}Ni_{0.81}$ alloy are centred around 0.04 and 0.20 Ry below E_F [35, 6]. Our results for $Cu_{0.2}Ni_{0.8}$ show that these energies are 0.03 and 0.18 Ry, respectively. They are better than the values 0.01 and 0.12 Ry obtained within the CPA-KKR for this alloy [6].

Comparing the APW-VCA results with the CPA ones it should be noted that the CPA result, in particular the shape of the $N(E)$ curves near the Fermi energies, is very sensitive to the choice of the splitting parameter δ, determining the energy interval between the d-scattering resonances of the different atoms, and the highest sensitivty takes place at low contents of transition metals. This parameter is free, so for CuNi alloys it was 0.134 Ry [1], or varied in the range from 0.107 up to 0.112 Ry for different concentrations [6]. For AgPd alloys δ changed from 0.150 up to 0.164 [2]. The extreme sensitivity to δ was mentioned in the KKR-CPA method too [6]. In the present work this energy interval is calculated and is equal to 0.121 Ry for CuNi and 0.240 Ry for AgPd alloys.

The obtained values of the density of electronic states at the Fermi energy $N(E_F)$ were used for the calculation of the low temperature specific heat coefficient γ through the relation

$$\gamma = \frac{\pi^2 k_B^2}{3} N(E_F)(1+\lambda), \tag{8}$$

where λ is known as the electron mass enhancement factor. As factor λ the following empirical values 0.14, 0.3, 0.1 and 0.7 were taken for Cu, Ni, Ag and Pd, respectively [29]. A linear dependence $\lambda(x)$ for the alloys considered here was assumed. The calculated dependencies $\gamma(x)$ as functions of alloy concentration are presented in Fig. 2a and 3a. The results within the CPA [1, 7, 9] and the experimental values [36, 37] are presented here too. As a whole the agreement of calculated specific heat coefficient $\gamma(x)$ with the experiment may be considered as satisfactory. The significant deviation from the experimental dependence for copper-nickel alloys takes place near the ferromagnetic phase transition, because we ignored the ferromagnetic ordering.

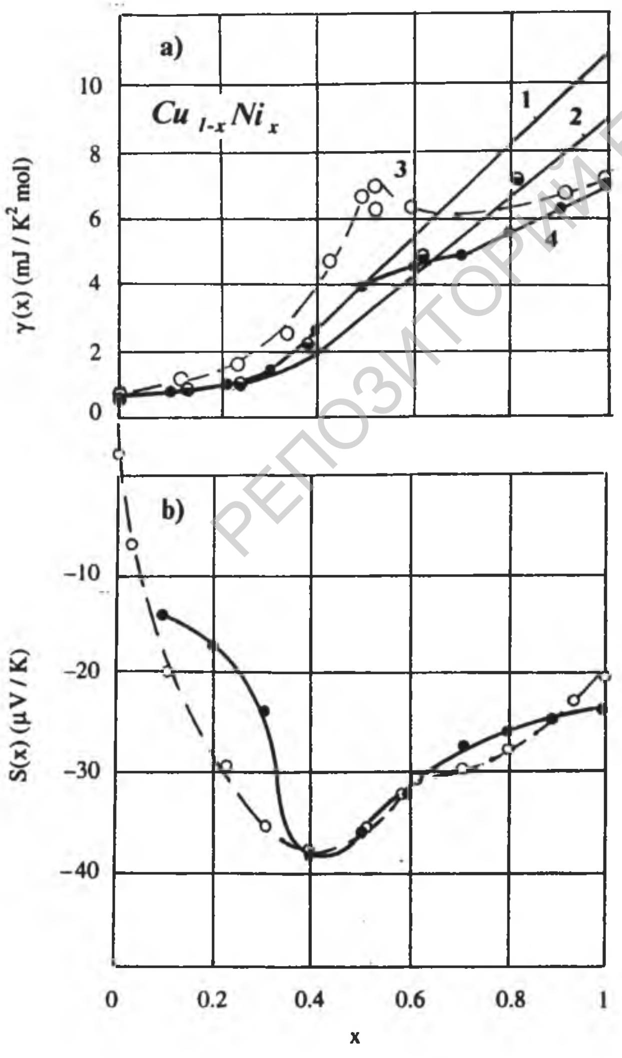

Fig. 2. a) The electronic specific heat coefficient for $Cu_{1-x}Ni_x$ alloys. Curves 1 and 2 are the results of TB-CPA [1], curve 3 (open circles) represents experimental data [36], curve 4 (solid circles) shows the present work (APW-VCA), the half-shaded circles are the KKR-CPA results [7]. b) The diffusion thermopower for $Cu_{1-x}Ni_x$ alloys. Full line (solid circles), present results for $T = 50$ °C; dashed line (open circles), experimental dependence, measured for the temperature interval 0 to 100 °C [23]

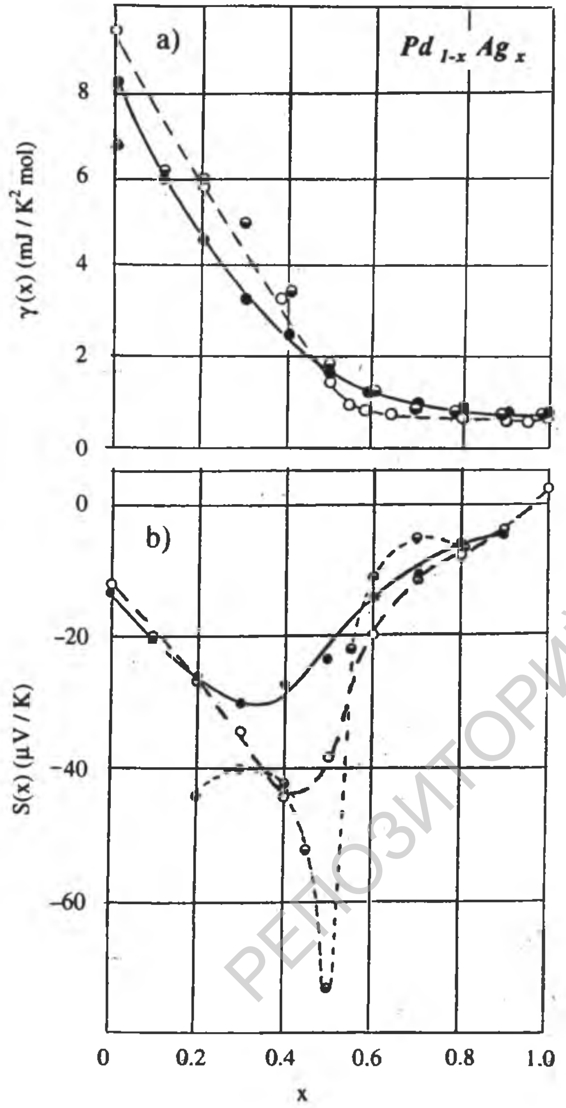

Fig. 3. a) The electronic specific heat coefficient for Ag_xPd_{1-x} alloys. Full line (solid circles), present results (APW-VCA); half-shaded circles, TB-CPA results [9]; open circles, experimental data [37]. b) The diffusion thermopower of Ag_xPd_{1-x} alloys for $T = 100$ °C. Full line (solid circles), present calculation; half-shaded circles, KKR-CPA results [5]; dashed line (open circles), experimental data [38]

The diffusion thermopower S is calculated from the expression (4). The derivative of the density of states at the Fermi energy $(dN/E)_{E_F}$ is evaluated by approximating the dependence $N(E)$ close to E_F by a parabola. The interval of differentiation was being decreasing until the derivative at the left and at the right of E_F began to coincide with an accuracy of the fifth digit. The results are shown in Fig. 2b and 3b for the temperatures $T = 50$ °C (Cu–Ni) and $T = 100$ °C (Ag–Pd). The dashed lines represent the experimental dependencies $S(x)$ for Cu–Ni alloys measured in the temperatures interval 0 to 100 °C [23], and for Ag–Pd alloys at $T = 100$ °C [38]. The available results of the KKR-CPA [5] for the diffusion thermopower are shown here too, they are reduced to the same temperature. It is obvious that our curve better correlates with the experimental ones. The deviation from the experiment is connected, in our opinion, first of all with the non-self-consistency of the APW method used for calculation of the electronic structure in pure metal components. That is why for Cu–Ni alloys, for which the initial approach was chosen more successfully, the best agreement with experiment is obtained.

Thus, Schoen's augmented-plane-wave virtual-crystal approximation allows one to obtain quite satisfactory agreement with experiment in the calculation both of the electronic energy spectra and concentration dependence of electronic properties of disordered alloys in the whole range of concentration. The results are in quantitative accordance with the experiment without adjustable parameters.

References

[1] G. M. Stocks, R. W. Willams, and J. S. Faulkner, Phys. Rev. B **4**, 4390 (1971).
[2] G. M. Stocks, R. W. Willams, and J. S. Faulkner, J. Phys. **3**, 1688 (1973).
[3] H. Ehrenreich and L. Schwartz, Solid State Phys. **31**, 150 (1976).
[4] J. S. Faulkner, Progr. Mater. Sci. **27**, 1 (1982).
[5] W. H. Butler and G. M. Stocks, Phys. Rev. B **29**, 4217 (1984).
[6] G. M. Stocks, W. M. Temmerman, and B. L. Gyorffy, Phys. Rev. Lett. **41**, 339 (1978).
[7] B. E. A. Gordon, W. M. Temmerman, and B. L. Gyorffy, J. Phys. **11**, 1821 (1981).
[8] A. J. Pindor, W. M. Temmerman, B. L. Gyorffy, and G. M. Stocks, J. Phys. **10**, 2617 (1980).
[9] P. M. Laufer and D. A. Papaconstantopoulos, Phys. Rev. B **35**, 9019 (1987).
[10] R. Richter, H. Eschrig, and B. Velicky, J. Phys. **17**, 351 (1987).
[11] J. M. Schoen, Phys. Rev. **184**, 858 (1969).
[12] R. H. Parmenter, Phys. Rev. **97**, 587 (1955).
[13] J. M. Schoen and S. P. Denker, Phys. Rev. **184**, 864 (1969).
[14] V. M. Golub and A. S. Karolik, Vestnik Akad. Nauk Belarus, Ser. Fiz.-Mat. Nauk No. 2, 87 (1995).
[15] F. J. Blatt, P. A. Shroeder, C. L. Foiles, and D. Graig, Thermoelectric Power of Metals, Plenum Press, New York/London 1976.
[16] I. A. Abrikosov, Yu. H. Vekilov, and A. V. Ruban, Dokl. Akad. Nauk SSSR **315**, 593 (1990).
[17] V. E. Panin and V. P. Fadin, Phil. Mag. **18**, 1301 (1968).
[18] M. V. Vedernikov and V. G. Dvunitkin, Fiz. Tverd. Tela **20**, 3302 (1978).
[19] R. Fletcher and D. Greig, Phil. Mag. **17**, 21 (1968).
[20] Sh. Sh. Abelskii, N. V. Ryanova, and U. P. Irchin, Fiz. Metallov i Metallovedenie **57**, 408 (1984).
[21] L. L. Kiang and T. L. Lin, Nuovo Cimento Lettere **18**, 41 (1977).
[22] N. F. Mott, Proc. Roy. Soc. A **156**, 368 (1936).
[23] B. R. Colles, Proc. Phys. Soc. B **65**, 221 (1952).
[24] P. A. Shroeder, R. Wolf, and J. A. Woollam, Phys. Rev. A **1**, 105 (1965).
[25] J. M. Ziman, Adv. Phys. **37**, 1 (1961).
[26] J. Yamashita and S. Asano, Progr. Theor. Phys. **50**, 1100 (1973).
[27] A. A. Lukhvich and A. S. Karolik, Fiz. Metallov i Metallovedenie **59**, 1085 (1985).
[28] E. Clementi and C. Roetti, Atomic Data and Nuclear Data Tables **14**, 177 (1974).
[29] P. Rennert and G. Paasch, in: Ergebnisse in der Elektronentheorie der Metalle, Ed. P. Ziesche and G. Lehmann, Akademie-Verlag Berlin 1983.
[30] G. Lehmann and M. Taut, phys. stat. sol. (b) **54**, 469 (1972).
[31] A. S. Karolik and V. M. Golub, Vesci Akad. Navuk Belarusi, Ser. Fiz.-Mat. Navuk No. 4, 96 (1997).
[32] A. S. Karolik and V. M. Golub, Fiz. Metallov i Metallovedenie **85**, 6 (1998).
[33] S. Hufner, G. Wertheim, and J. Wernick, Phys. Rev. **8**, 4511 (1973).
[34] J. Hedman, M. Klasson, R. Nilsson, C. Nordling, M. F. Sorokina, O. I. Kljushnikov, S. A. Nemnonov, V. A. Trapeznikov, and V. G. Zyryanov, Physica Scripta **4**, 195 (1971).
[35] D. H. Seib and W. E. Spicer, Phys. Rev. B. **2**, 1676 (1970).
[36] K. P. Gupta, C. H. Cheng, and P. Beck, Phys. Rev. A **133**, 203 (1964).
[37] H. Montgomery, G. P. Pells, and E. M. Wray, Proc. Roy. Soc. A **301**, 261 (1967).
[38] A. A. Rudnitskii, Termoelektricheskie svoistva blagorodnykh metallov i ikh splavov, Izd. Akad. Nauk SSSR, Moscow 1956.