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On the Electronic Structure of Phosphorus in Nickel

By

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The electronic density of states of the Ni–P amorphous system is calculated in a self-consistent way from first principles, using a KKR Green's-function method with a single perturbed muffin-tin potential in a periodic lattice.

Aus den ersten Prinzipien wird die elektronische Zustandsdichte des amorphen Ni–P-Systems selbstkonsistent mit einer Green-Funktionen-KKR-Methode und einem einzigen gestörten „muffin-tin“-Potential in einem periodischen Gitter berechnet.

1. Introduction

Special interest has been focused more recently on nickel–phosphorus amorphous systems, mainly on their wide range of industrial application. The basic physical problem is connected with the electronic structure of these alloys, namely with the charge transfer, the possible forms of the electronic hybridization of the components, the speciality of valence band, etc. The results obtained by different theoretical methods are not at all consistent. According to the rigid-band model [1] a massive charge transfer is expected from phosphorus to nickel, filling up the empty states of the Ni 3d-band by 3p-electrons of P. At the same time, the LCAO calculations resulted an opposite charge transfer: from Ni to P at about $0.5e$ (e is the denotation of an electron) [2]. Moreover the results of LMTO calculations are entirely different, showing a considerable (about $1.42e$) charge transfer from P to Ni [3]. Recently the results obtained by other calculations as by the KKR-CPA method [4] and by cluster calculation with the discrete variational method (DVM) [5] concluded to the impossibility of the donor-like role of phosphorus in these systems. The experiments, on the other hand, did not verify the rigid-band calculations, reporting a slight change only in E_F as well as in the d-holes in the system Ni–P [6]. The absence of charge transfer was supported by other experiments [7] as well, when no significant charge transfer was observable; only the hybridization of s- and p-electronic states of phosphorus with Ni 3d-states was dominant.

The various calculations have several disadvantages; the cluster calculations have problems with the finite cluster size and with its extension, surfaces, etc. Similarly the supercell calculations are problematic because, if a certain structure contains a defect,

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it will be repeated through the whole crystalline structure, invoking a periodically arranged effect.

According to these earlier discussions the real electronic structure of the system NiP is not clarified in details yet, and the questions related to it are relevant.

An ab-initio calculation applying the Kohn-Karringa-Rostocker Green's function method (KKR-GFM) is presented here.

We have worked out a new version of the method KKR-GFMT (KKR Green's function muffin-tin) in the frame of the approach LAPW for the electronic structure of phosphorus in Ni matrix. The impurity is described by a single perturbed muffin-tin (MT) potential in an infinite periodic lattice. The Green's function method describes correctly a single perturbation in an infinite crystal, and the condition of self-consistency can also be met easily applying it. All of the disadvantages of other methods could be avoided by this calculation since it supposes that the full spatial extent of the perturbed potential is localized.

We try to discuss several problems of a system with small amount of phosphorus, as an impurity in a Ni-matrix. We expect that upon dilution the interaction between phosphorus atoms will be negligible and the density of electronic states $[N(E)]$ will be the same as in the processes of alloying for the more complicated concentrated systems. The effect on $N(E)$ by phosphorus as well as the more general behaviour of the impurity-like states have been presented in our present paper. It is shown that all those relevant effects on the electronic structure appear in these dilute alloys which are important in the concentrated ones.

The calculation are based on the Green's function of defect crystalline state constructed by the linear augmented plane wave (LAPW) method [8].

2. The Method of Calculation

The method of Green's function is well developed [9, 10] for the electronic structure of defects in homogeneous matrices [11 to 15]. In many cases the KKR method [16] has been applied. There are some difficulties connected with this method such as the discontinuity of basic wave functions and the necessity of singularity on KKR structure constants [9].

In the present paper the LAPW method has been used, which had been successfully applied in calculations of electronic structures and optical properties of various compounds [17 to 20].

Let us start with the spectral form of the Green's function [10],

$$G(r, r', E) = \frac{\Omega_0}{(2\pi)^3} \sum_{\lambda} \int_{\text{B.Z.}} \Psi_{k\lambda}(r) \Psi_{k\lambda}^*(r') (E - E_{k\lambda})^{-1} dk, \quad (1)$$

where r and r' are radius vectors, Ω_0 is the volume of the Wigner-Seitz cell, E , λ , and k are the energy, zone index, and wave vector, respectively; the integral is taken over the whole Brillouin zone. $\Psi_{\lambda k}(r)$ and $E_{k,\lambda}$ are the wave function and self-energy as generally used in the KKR method. Used the solution of Schrödinger's equation in MT-sphere the $G(r, r', E)$

function has been presented by a standard way [21 to 22],

$$G(r + R^n, r' + R'^n; E) = -i\delta_{mn',k} \sum_L R_L^n(r, E) Y_L(r) H_L^n(r_>, E) Y_L(r') \\ + \sum_{LL'} R_L^n(r, E) Y_L(r) G_{LL'}^{mn'}(E) R_L'^n(r', E) Y_{L'}(r'); \quad (2)$$

$$r_> = \max(r, r'), \quad r_< = \min(r, r')$$

with the notations

$Y_L(r)$ spherical harmonics,

$L = (l, m)$ orbital quantum numbers,

R^n and R'^n atomic positions,

$K = \sqrt{E}$; $H_L^n(r; E) = R_L^n(r, E) + iN_L^n(r, E)$,

$N_L^n(r, E)$ nonregular solution of the radial Schrödinger equation,

$G_{LL'}^{mn'}(E)$ energy-dependent coefficients of the Green's function.

The solution of Schrödinger's equation for $R_L^n(r, E)$ and $H_L^n(r, E)$ satisfies the following conditions:

$$R_L^n(r, E) = j_l(k, r) - i\sqrt{E} t_l^n(E) h_l(k, r), \quad (3)$$

$$H_L^n(r, E) = h_l(k, r),$$

where $j_l(k, r)$ is the spherical Bessel function, $t_l^n(E)$ is the scattering matrix in the n -th MT-sphere, which is calculated by the standard method, used the phase shifts of scattering [9 to 10], and $h_l(k, r)$ is a first order spherical Hankel function.

The perturbations caused by defects in a real crystal can be considered as a modification of the ideal crystalline state ($G_{LL'}^0(E)$, [10]),

$$G_{LL'}^{mn'}(E) = G_{LL'}^{0mn'} + G_{LL''}(E) \Delta t_l^{n''}(E) G_{L''L'}^{n''m'}(E), \quad (4)$$

where $\Delta t_l^{n''}$ is the change in the scattering of the matrix.

In the case of a distortion of the potential taken into account only in one MT-sphere and only the s-, p- and d-phase shifts are used for calculations, then (4) has been reduced to four scalar conditions,

$$G_{LL}^{mn}(E) = \frac{G_{LL}^{0mn}(E)}{1 - G_{LL}^{0mn}(E) \Delta t_l^n(E)}. \quad (5)$$

Using the coefficients obtained, the density of electronic states in the MT-sphere becomes [23] as follows:

$$N(E) = -\frac{2}{\pi} \int_{V_T} \text{Im} G(r, r'; E) dr \quad (6)$$

and the corresponding electron density is

$$n(r) = -\frac{2}{\pi} \int_{-\infty}^{E_F} \text{Im } G(r, r; E) dE. \quad (7)$$

A self-consistent iteration-process has been introduced for the calculation of the density of electronic states. For the calculation of the bulk potential Vosko's parametrization [24] has been used. The charge transfer into the MT-sphere has been calculated by the density of electronic states obtained before.

Within the LAPW method the representations of the wave function are

$$\begin{aligned} \Psi_{k\lambda}(r) &= \sum_i a_i^{k\lambda} \varphi_{ki}(r), \\ \varphi_{ki}(r) &= \begin{cases} \frac{1}{\Omega_0} \exp(ikr); & r > R_s, \\ \frac{4\pi R_s^2}{\sqrt{\Omega_0}} \exp(ik_i \tau_s) \sum_L i^l \varphi_L^s(k_i r) Y_L(r) Y_L^*(k_i); & r \leq R_s, \end{cases} \\ \varphi_L^s(k_i, r) &= a_{sli} R_{sl}(E_{sl}; r) + l_{sli} \frac{dR_{sl}(E_{sl}, r)}{dE}, \end{aligned} \quad (8)$$

where $a_i^{k\lambda}$ is the solution of the secular equation in the LAPW method, $k_i = k + b_i$; b_i is the reciprocal vector, R_s the radius of the s -type MT-sphere, τ_s the position of the MT-sphere in the elementary cell, a_{sli} and b_{sli} are coefficients determined by fitting the wave vectors on the surface of the MT-sphere, $R_{sl}(E_{sl}, r)$ come from the solution of the radial Schrödinger equation in the s -th MT-sphere with energy E_{sl} , normalized as

$$\int_0^{R_s} r^2 dr R_{sl}^2(E_{sl}) = 1. \quad (9)$$

The function $\Phi_L^s(k_i, r)$ depends indirectly on the energy through the wave vector k . The direct substitution of $\Phi_L^s(k_i, r)$ into (2) is not possible. By the substitution (8) into (1) and used (2), after an integration, we obtain

$$\begin{aligned} G_{LL'}^{nn'} \alpha_{ll'}^{nn'}(E) &= i \delta_{nn'} \delta_{LL'} k \alpha_{ll'}^{nn'}(E) |\alpha_{ll'}^{nn'}(E)| \\ &\quad - 2R_s^2 R_s'^2 \sum_{\lambda} \int_{\text{BZ}} i^{l-l'} (E - E_{k\lambda})^{-1} dk \sum_{i,j R_s} a_i^{k\lambda} (a_j^{k\lambda}) \\ &\quad \times \exp(i[k_i R^n - k_j R^{n'}]) \int_0^{R_s} \Phi_L^s(k_i, r) R_l^n(r, E) r^2 dr \\ &\quad \times \int_0^{R_s'} \Phi_{L'}^s(k_j, r) R_{l'}^{n'}(r, E) r^2 dr Y_L^*(k_i) Y_{L'}(k_j), \end{aligned} \quad (10)$$

where

$$\alpha_{ll'}^{ss'}(E) = \int_0^{R_s} R_l^n(r, E) R_{l'}^{n'}(r, E) r^2 dr. \quad (11)$$

Using the following approximation for $R_l^n(r, E)$:

$$R_l^n(r, E) = \left(R_{sl}(E_{sl}, r) + (E - E_{sl}) \frac{dR_{sl}(E_{sl}, r)}{dE} \right) \left(\frac{\alpha_{ll}^{ss}(E)}{1 + (E - E_{sl})^2 N_{sl}} \right)^{-1/2}, \quad (12)$$

where

$$N_{sl} = \int_0^{R_s} \left(\frac{dR_{sl}(E_{sl}, r)}{dE} \right)^2 r^2 dr,$$

finally we get

$$\begin{aligned} \text{Im} [G_{LL'}^{mn'}(E) \sqrt{\alpha_{ll'}^{ss}(E) \alpha_{l'l}^{s's'}(E)}] &= \delta_{mn'} \delta_{LL'} k |\alpha_{ll}^{ss}(E)| - 2R_s^2 R_{s'}^2 \\ &\times \sum_{\lambda} \int_{\text{BZ}} \delta(E - E_{k\lambda}) dk_i^{l-l'} \sum_{ij} a_i^{k\lambda} (a_j^{k\lambda})^* \\ &\times \exp(i[k_i R^n - k_j R^{n'}]) (a_{sli} + (E - E_{sl}) b_{sli} N_{sl}) [1 + (E - E_{sl})^2 N_{sl}]^{-1/2} \\ &\times (a_{s'l'j} + (E - E_{s'l'}) b_{s'l'j} N_{s'l'}) [1 + (E - E_{s'l'})^2 N_{s'l'}]^{-1/2} Y_L^*(\hat{k}_i) Y_{L'}(\hat{k}_j). \end{aligned} \quad (13)$$

In the concrete calculation performed for Ni the self-consistent potential calculated by LAPW has been used, with the integrals in (13) approximated by a tetrahedral algorithm with quadratic interpolation. In fact, the set of the basis functions calculated by this method is not complete,

$$\Psi_{k,\lambda}(r) = \hat{P} \bar{\Psi}_{k,\lambda}(r), \quad (14)$$

where P is a projection operator applied to $\bar{\Psi}_{k,\lambda}(r)$, which is the exact single electronic wave function of the crystal. Any exact solution must satisfy the sum rule [25] and other a priori conditions [26]. It is easy to prove that the better the sum rules are obeyed, the better is the reliability of the Green function coefficients in (2). This is realized when the set of basic functions is almost complete.

Consequently, we expect a small error only at the transition from the LAPW basis to the KKR case [27, 28]. A further control of the feasible determination of the imaginary part of the Green function is its comparison with the density of electronic states calculated by LAPW in (5).

The real part of the Green's function can be calculated by the Kramers-Kronig relation

$$\text{Re} G_{LL'}^{mn'}(E) \alpha_{ll'}^{ss'}(E) = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im} G_{LL'}^{mn'}(E') \alpha_{ll'}^{ss'}(E') dE'}{(E - E')}. \quad (15)$$

In order to carry out the calculation in an appropriate number as well as cut of energy boundaries for the evaluation of the integral in (15) a lot of points in the energy space are required. As a consequence, a regular calculation of Kramers-Kronig's transition needs a lot of computer time. To reduce the requirements, the real part of the Green's function was calculated by Gilber's transformation [29] employing quick Fourier transformation.

One of the most important questions in our present work is the validity and limitations of the presented approximation of a strongly localized model calculation (SLMC) of defects. The real physical properties have to be investigated concretely, how they are approximated when taking into consideration only the localized interactions between the impurity and matrix atoms in their near vicinity. The case having larger and larger number of atoms involved obviously offers better and better approximations to the real situation. The

Table 1

Comparison of the total momentum of the cluster containing the impurity and its twelve neighbours for some selected 3d-metal impurities in Cu

impurity	calculations		present	experiments
	[30]	[31]		
Cr	3.39	3.30	3.66	2.46 [32]
				3.9 [33]
Mn	3.65	3.58	3.68	3.96 [32]
				4.93 [34]
Fe	2.62	2.51	2.76	3.68 [35]
				3.4 [36]
				3.0 [37]

difficulties of the technical computational problems generated by this condition are not proportional with the value of the information reached by the procedure. There are a few calculations for the magnetic defects (3d-metals) considering a large number of coordination shells involved [30, 31] in copper matrix. These calculations for the total magnetic moment are repeated by the present method for Cr, Mn, and Fe impurities in Cu. Our results, in comparison to others, are given in Table 1.

Despite of our very simple calculation the correspondence with the other results is satisfying, moreover the agreement with experimental data is better in our case. Furthermore, using these principles for calculations of electric resistivity also is well fitting to experiments [38]. There is another qualitative probe of the effectivity of SLMC, the comparison of the charge of the impurity and an ideal matrix atom in the MT-spheres. For the 3d-impurities (in paramagnetic state) there are the charge values in Cu matrix as follows: Sc - 0.52, Ti - 0.45, V - 0.35, Cr - 0.25, Mn - 0.16, Fe - 0.08, Co - 0.01, Ni - (-0.04). These values are so small that the localized considerations are not contradicting in this point. In the case of phosphorus defects in Ni matrix we have no (calculated or measured) information, but in this case the charge in the MT-sphere of P is also not large in comparison to the charge of the Ni matrix in their MT-sphere. These are the charge transfers 0.32, 0.31 and 0.24 in the cases of Ni (f.c.c.), Ni (b.c.c.), and Ni (cub.) respectively. This small effect is also giving reality to the localized approach of the system. The reasonable agreement between cluster and band structure calculations for metall-metalloid systems [39] is also supporting the validity of our present calculations.

3. Results and Their Discussion

The partial density of electronic states (PDOS) for pure f.c.c. Ni calculated by our method is given in Fig. 1. In the vicinity of the Fermi energy the d-states are characteristic. The d-zone has hole states which is a necessary condition for d-sp hybridization.

As deduced from experiments [7], the electronic structure of pure Ni changes but slightly due to the phosphorus alloying. For understanding the role of P in Ni, we have calculated the PDOS of P in Ni (f.c.c.) matrix (Fig. 2). In comparison with the PDOS of pure Ni, the hybridization of sp-states of P with d- and p-states of Ni is well observable. While p-states of P and d-states of Ni are overlapping, the PDOS of p-states of phosphorus at the top of the valence band is small. The basic interaction appears between the hybridized

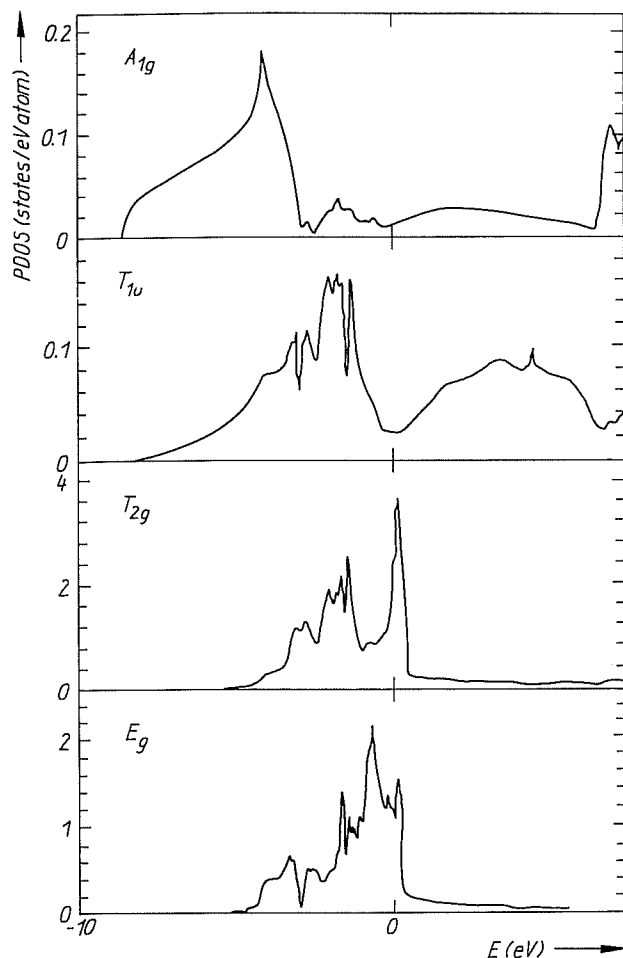


Fig. 1. PDOS of pure f.c.c. Ni

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sp-states of Ni and sp-states of phosphorus. In the region of 7 to 10 eV below E_F the impurity-states of P are clearly seen. Finally, antibonding states of P are formed 7 to 8 eV above E_F , mainly consisting of p-states.

The main question is the direction and amount of the charge transfer, which can also be calculated in our approximation. We have got about $0.32e$ charge transfer from P to Ni, which is pretty small and not against the experiments [40]. For the more concentrated alloys, the P-P interaction will further reduce this charge transfer value since it was calculated for an isolated impurity.

In the formation of the amorphous state a number of different clusters (Ni_mP_n) must also be considered; so the influence of the nearest neighbourhood (with a given symmetry and composition) on density of electronic states (DOS) would become important.

Based on these ideas various hypothetical structures (such as b.c.c. nickel, cubic nickel) and the impurity states of P in them have been calculated by using the present method. In the first step the pure hypothetical b.c.c. Ni and cub. Ni have been calculated (Fig.3). Contrary to the results for the f.c.c. Ni calculation (Fig. 4) characteristic differences could be observed

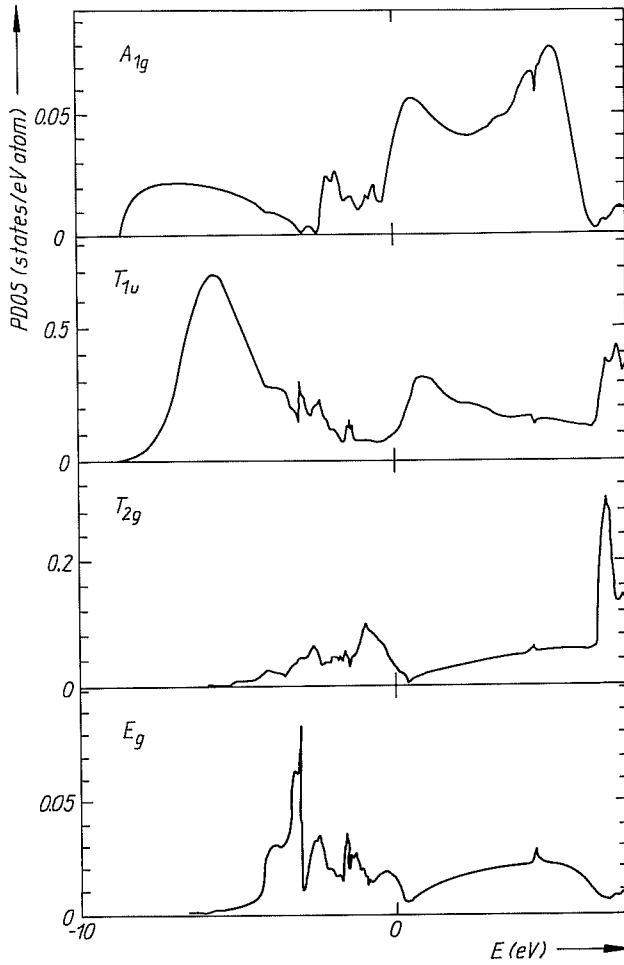


Fig. 2. PDOS of P in f.c.c. Ni

at the vicinity of E_F . In the case of the amorphous structure we can assume that short range symmetries exist, and a mixed, weighted average of PDOS is seen in the PDOS of the hypothetical amorphous pure Ni, taking into consideration the requirement of equality of Fermi energies, during the averaging. As a first approximation the common band can be constructed by the rigid shift of the obtained DOS curves to an acceptable E_F energy, very close to E_F for f.c.c. Ni. In this shifted case several similarities between these DOS curves belonging to different local symmetries become clear. The calculation has been made for P impurity in the hypothetical b.c.c. and cubic symmetries.

The PDOS for P in b.c.c. Ni (Fig. 5) is very similar to the PDOS for P in f.c.c. Ni (see Fig. 2). The result of calculations for $N(E)$ is shown on Fig. 6. The calculated charge transfers for f.c.c., b.c.c., and cubic structures are $0.32e$, $0.31e$, and $0.24e$, respectively. The s-states of P are slightly changing in an interval of 7 to 10 eV below E_F and the change is more considerable at the top of the valence band. This causes a larger sp-hybridization of P and the interaction of sp-states of P with Ni d-states. Due to the relatively large density and delocalization of P p-states the symmetry change is more effective for this state than for others. On the other hand, the calculated $N(E)$ for different hypothetical symmetries are

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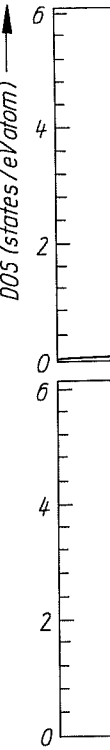
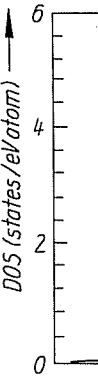
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DOS of P in f.c.c. Ni

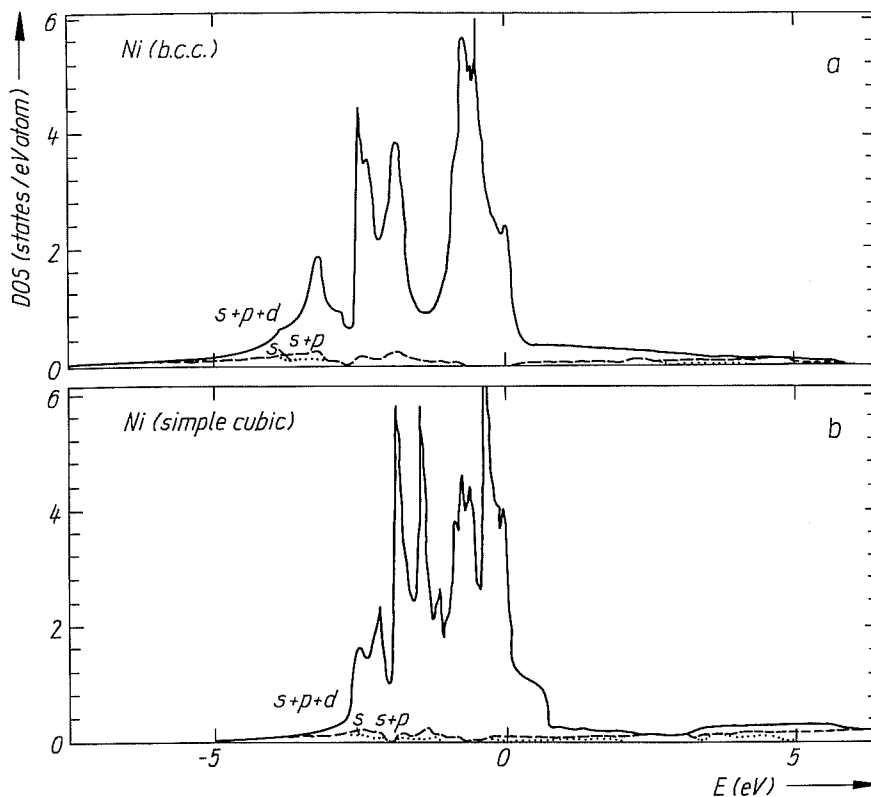


Fig. 3. Hypothetical DOS of Ni. a) B.c.c. structure, b) simple cubic structure

not so different from each other as far as their shape is regarded. It reflects the main behaviour of the P impurities in Ni matrix, and accounts for various hybridizations of P and Ni states. The energies of bonding states of P are changing only slightly with 12.2, 11.65, and 10.2 eV below E_F for f.c.c., b.c.c., and cubic structures, respectively.

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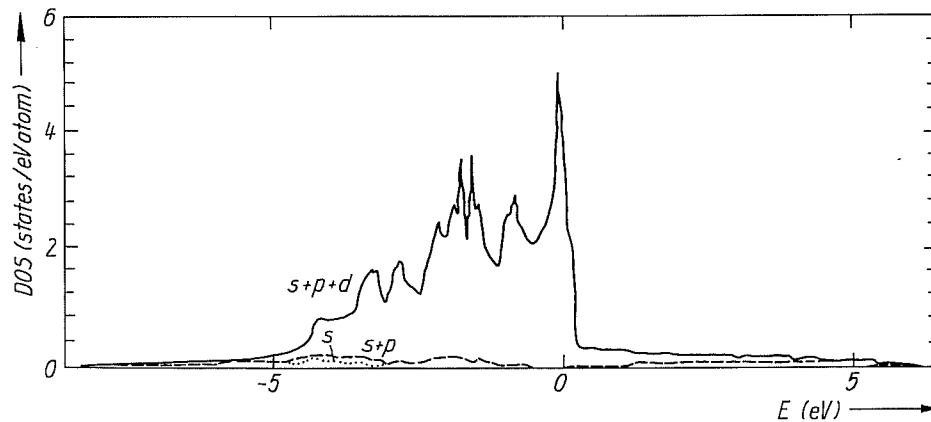


Fig. 4. DOS of pure f.c.c. Ni

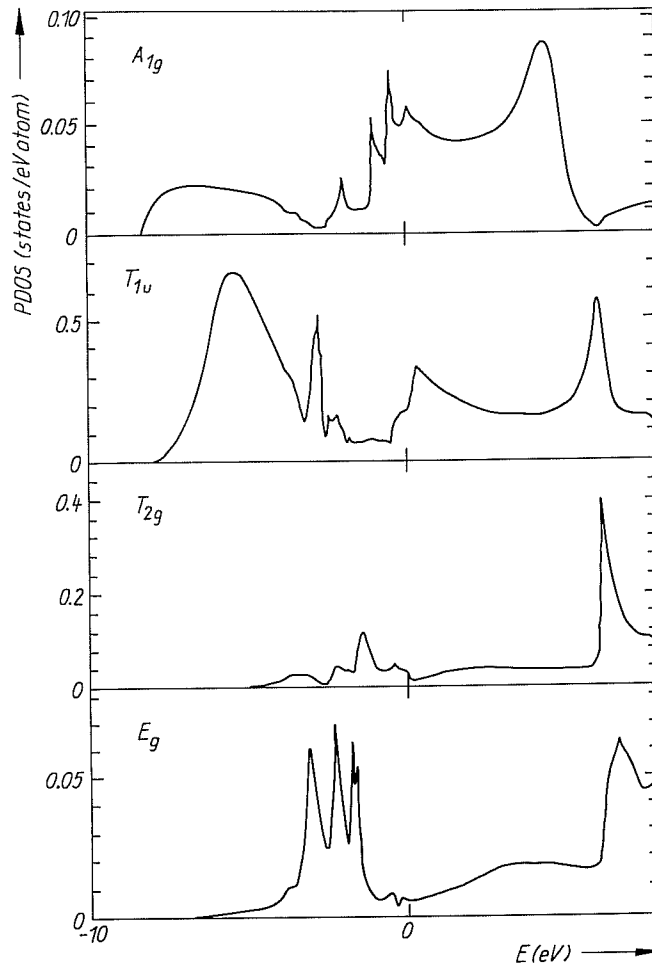


Fig. 5. PDOS of P in b.c.c. Ni

Constructing the amorphous state an average can be assumed. Since the differences in $N(E)$ are not so large for different cases of symmetry, we can assume that the first coordination sphere with its special short-range order and symmetry does not influence so much the electronic structure of the amorphous state as was expected. On the other hand, the electronic structure has an important role in stabilizing the Ni-P system [41 to 43], so the effect of second and further coordination spheres should be important as well. It means that in the case of this system the medium-range order should be of basic importance, as has been discussed before [44].

4. Conclusion

An LAPW method in the frames of the Green's function formalism was developed for the calculation of electronic structure of phosphorus impurity in hypothetical crystalline modifications of Ni. It was shown that only a small charge transfer from P to Ni appears in the case of single P impurity, which becomes smaller at increasing phosphorus concentration.

Fig. 5. PDOS of P in b.c.c. Ni

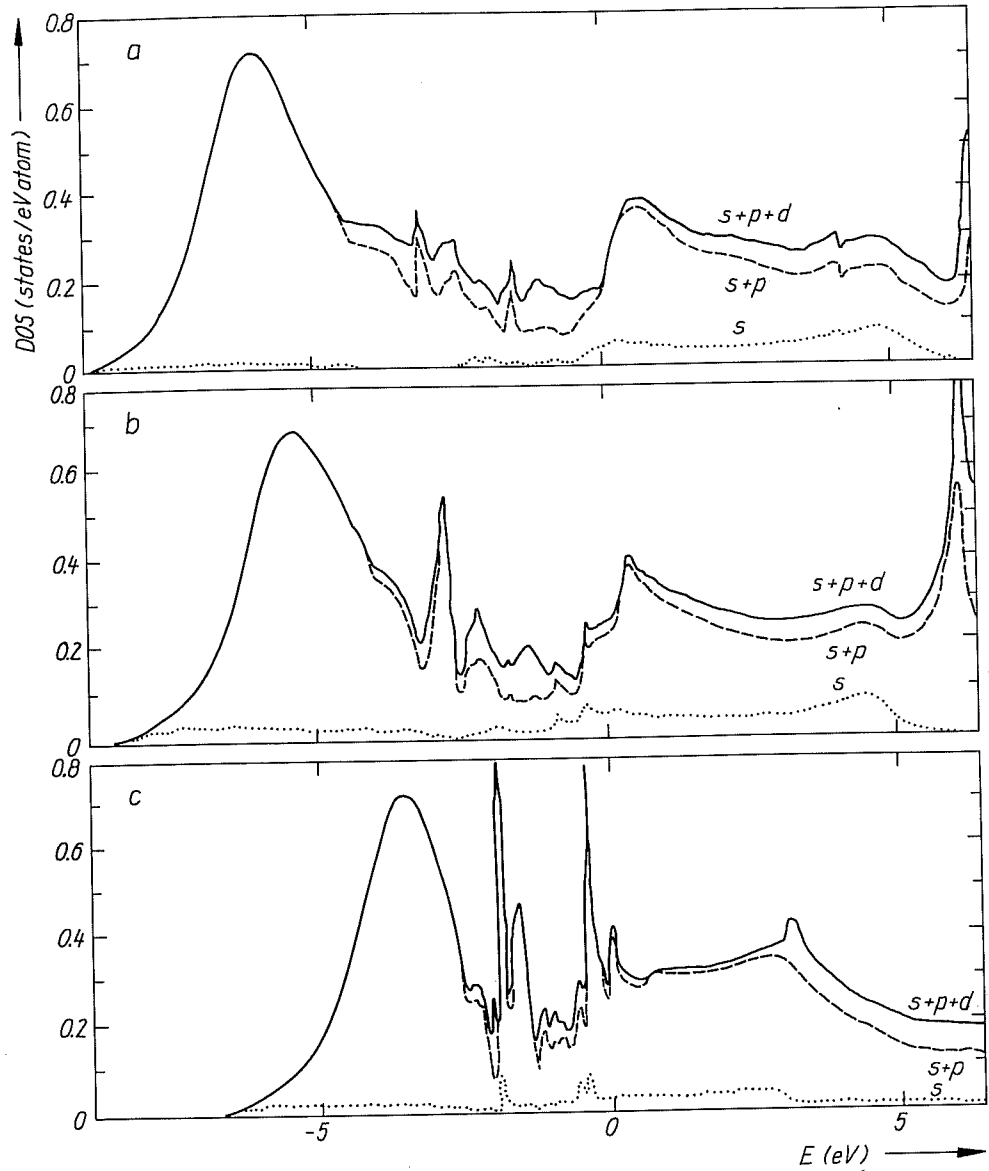


Fig. 6. DOS of P in different structures of Ni. a) F.c.c. Ni, b) b.c.c. Ni, c) cubic Ni

Since the differences in $N(E)$ that the first coordination influence so much the electronic structure [43], so the effect of second coordination means that in the case of this has been discussed before

ism was developed for the synthetic crystalline modification P to Ni appears in the phosphorus concentration.

We could not observe any appreciable charge transfer in the Ni-P system. Less essential differences were observed between the electronic structures of Ni-P systems with different short-range symmetries. The evaluation of these facts leads to the conclusion, that the medium-range symmetries have an important role in stabilizing the Ni-P amorphous system. The investigation of this topic is in progress.

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