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Chapter 13

Properties of the Ultrathin Multilayer Ground State of Fe/Pd

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Additional information is available at the end of the chapter

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Abstract

The technological evolution in the recent years allowed us to improve computers. Consequently, the numeric calculus with computational methods had a big progress. In theoretical physics that had a benefit with this technology, we can highlight the calculation of the solids' electronic structure. Using the first principles method, LMTO (Linear Muffin-Tin Orbital) with the ASA (Atomic Sphere Approximation) approximation, we will study the band structure in the magnetic multilayers. The choice of these methods was based on two aspects: (a) The computer available to perform the job; a CRAY super computer that belongs to the Supercomputer National Center. Because the LTMO method presents good vectorization, it allows us to perform calculations with many atoms in the unitary cell, which would be too difficult with a smaller computer. (b) The fact that the LMTO method already presented good results in studies like intermetallic alloys and of iron nitride substituted.

Keywords: Band structure, calculation of the first principles, Ultrathin Multilayer

1. Introduction

1.1. Calculation of band structure: A brief history

In this section, a brief history of the calculation of band structure is provided, invoking the main methods used in this way. This does not intend to supplement, but to give the reader a good basis, especially for those who are not experts in the area, to understand the concepts used in this chapter. The understanding of the distribution of electrons in solids gives an appreciation of some of their physical properties. The most interesting properties of the new material industry, such as magnetization, come from the distribution of electrons in a solid. Theoretically, we should treat a system of several electrons distributed randomly in the

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material. However, we cannot follow this infinite number, and we must use the Born-Oppenheimer approximation. We treated electrons and the nuclei as if they were separate from each other. So, we will calculate the energy of the ground state, depending on the position of the atomic nuclei. This implies that the basic problem is to calculate the steady states of the interacting electrons system moving in a periodic electrostatic field originated by the fixed nuclei i.e., to obtain the electronic structure of solids and consequently the structure of the same band. The identification of the electronic structure of solids involves considering an infinite number of the interacting fermions. But what does this mean? This leads us to solve the Schrödinger equation for an electron moving in an average field of other electrons over the field of the nuclei. Therefore, the field is determined by the distribution of the electronic charge, the adjustment for correlation, and the exchange effect. And it is usually calculated self-consistently as we shall see later on.

In the recent years and with the advent of powerful computers, which are faster and more accurate. Furthermore, the appearance of linear methods [01- 02] for calculating the structure of the ordered solid bands. We can see that some of the main calculation methods had a breakthrough. It comes from a theoretical but also a practical point of view because there was a technological breakthrough in providing fast and accurate computers. We can then identify the physical properties with greater ease and certainty of outcomes [05-06]. An important work of Hohenberg-Kohn-Sham [07-08] provides the theoretical base pair to the other methods because they teach us to work with the mean-field theory using the electron density function and the energy of the ground state.

Other methods have also emerged with the DVM [10] ("Discrete Variational Method"), SPR-LMTO [11] ("Spin Polarized Relativistic Linear Muffin-Tin Orbital"), and the FLMTO [12] (TUB Linear Muffin-Tin Orbital "). Currently, the first purest strains of methods are employed to study the defects in the crystal lattice [13].

The calculation of the first principles band structure is a very important tool in the study of thin films and multilayers. Such systems are investigated by different techniques, such as X-ray and Mossbauer duration or magnetization measurements [15-19].

In the modern calculation of the first principles applied to magnetic multilayers, Jarlborg and Freeman [21, 22]did some work that can be used as a primary reference. These calculations were motivated by the comments made by TJ Taler et al. [23] Ni / Cu alloys use ferromagnetic resonance. However, it should be considered that at that time, there was a difficulty in the experimental physics to build very thin layers (of the order 5-15 angstroms), which made the comparison between the calculations and the very difficult experience.

More recent studies using the first principles methods, such as performed by Blügel et al. [24] using the FLAPW ("Full Linear Augmented Plane Waves") that presented a good agreement with the experimental work carried out by Celinski et al. [19] In the case of magnetic multi-layers, in the recent years, there has been a promising advance in both the theoretical and experimental study, which can be checked in fairly comprehensive references on the subject [25]. However, it is necessary to continue the theoretical investigation of the magnetic properties and the structural ultrafine multilayer because there are still questions to be answered

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about the charge transfer, magnetic moments, and the "stress" in the interface region, which causes changes in the density of the states. Another problem to be studied is the multilayer stability into the very thin structures. Properties, such as the hyperfine field and isomer shift of multilayer stability, are also a point of interest. In this work, we will hold extremely thin multilayer calculations worrying about the interface region between the materials that make up the multilayer.

2. Introduction to calculate the electronic structure of ultrathin multilayers

In this chapter, we will investigate the magnetic properties of ultrathin multilayers and hyperfine Iron and Palladium (Fe / Pd). The multilayer research is done in a few different stoichiometries in order to have a better understanding of their magnetic properties and behavior in the pressure. We begin by studying the electronic structure of the ultrathin multilayers of Fe and Pd, with a composition of 50% of each element. Below, we will investigate the behavior of two different systems: the dual system ultrathin multilayers of iron and a palladium (2 Fe / Pd), and the inverse system (2 Pd / Fe). This enables a comparison between these three different systems, which will show a clear change in the band structure of the systems when we change its stoichiometric structure. The theoretical research for both Fe / Pd ultrathin multilayers, as in the case of the 2 Fe / Pd and 2 Pd / Fe systems, is made using the LMTO, method of Andersen [01-02], and approximation of the atomic spheres (ASA). To study the electronic structure of multilayer systems, in the ferromagnetic case, we performed the calculations with a spin polarization and the parameterization of von Barth and Hedin [36] for energy correlation and exchange of an electron gas. In the self-consistent calculations for the non-magnetic case, we used the Hedin-Lundqvist potential [34]. This LMTO calculation does not include the spin-orbit interaction as it is very small and put term fixes combined [01]. To solve the equation, Schrödinguer used the s atomic orbitals that present the results. We then started with the calculations of the structure of the Fe / Pd ultrathin multilayers.

3. Magnetic structure and electronics of the Fe/Pd ultrathin multilayers

Calculations were performed using a structural model in which the bilayers grow in the direction (0,0,1) with a packaging sequence ABA type with tetragonal structure. The ratio of the axes was c / a = 1.41 with the Fe atoms occupying the position (0,0,0) and Pd atoms at (0,1/2,1/2). We chose the muffin tin-spheres involving atoms with the same radius for both the Fe and the Pd atoms. We performed self-consistent calculations for various lattice parameters through which we obtained the amount of the theoretical equilibrium. Figure 1 shows the total energy as a function of lattice parameter for the ferromagnetic and nonmagnetic states. We noted that the stability of the ferromagnetic state in relation to the non-magnetic state is good because the energy difference in the volume balance between the ferromagnetic state and the non-magnetic is ΔE = -22.98mRy by atom. The lattice parameter in the balance was calculated using a third-degree polynomial, which was the best fit of the plotted points for both the

ferromagnetic state and the non-magnetic state. We obtained the lattice parameters a = 7,188u.a. for the ferromagnetic state and a = 7,044u.a. for the non-magnetic state. The value found for the ferromagnetic state is greater than the one found for the ordered alloy of 50% Fe and 50% Pd on self-consistent calculations. With the growth of the interatomic distances, Fe / Pd bilayers, and the consequent reduction of metal-metal interaction, such a system shows a slightly different magnetic behavior of the pure materials.

All tables are taken from the PhD thesis in reference 41. In table 1, we have the magnetic moment on the Fe site equal to 2,870μB in the Fe/Pd ultrathin multilayers. We noted that there was an increase in the magnetic moment on the website of Fe, compared to the pure iron that is 2,217μB [41].This is in agreement with the experimental work that measured the magnetic moments in the Fe / Pd multilayer [19].Here, we noticed a strong magnetic moment featuring a super magnetic alloy. In Table 1, it is easy to see that the greatest contribution of the electrons in the Fermi level N (E_F) is the electrons d-down the Fe site due to the loads transferred to this site.

	Fe			**Pd**		
	Up	**Down**	**Up - Down**	**Up i**	**Down**	**Up-Down**
N	5.4686	2.5986	2.8700	5.1563	4.7759	0.3804
n_s	0.3318	0.3275	0.0043	0.2824	0.2997	-0.0173
n_p	0.3718	0.3707	0.0011	0.3048	0.3326	-0.0278
N_d	4.7650	1.9004	2.8646	4.5691	4.1436	0.4255
$N(E_F)$	1.8851	13.8763		1.4616	3.5053	
$Nt(E_F)$		15.7614		4.9669		
NC(ef)				20.7283		
v				3.5924		
ΔQ		0.06744			-0.06744	
E_F				0.6532		

Table 1. Parameters calculated for the spin polarization ofFe / Pd bilayers using a self-consistent potential. Here, n is electron / spin; N in states / atom spin Ry; Nc states / Ry unit cell; y in mJ / molK2; EF Ry and ΔQ into electron.

4. Density states of the Fe/Pd ultrathin multilayers

The calculation of the density of states of d in the bilayers of the Fe and Pd sites are shown in Figures 2 and 3, respectively. We noted that there is a narrowing of the bands of the ultrathin multilayers compared to a league and the ordered FePd. Therefore, the metal-metal interaction causes a small change in the spin up and down states of the Fe and Pd metals. Figure 3 noted that the Pd site spin up and spin down states are busy unlike the one found for the DOS-d Fe site, which has many empty d spin-down states above the Fermi energy. In the Fe site, there are magnetic moments as the area below the Fermi energy is different between the up and down states, which is largely featuring a high magnetic moment in this place. This is in

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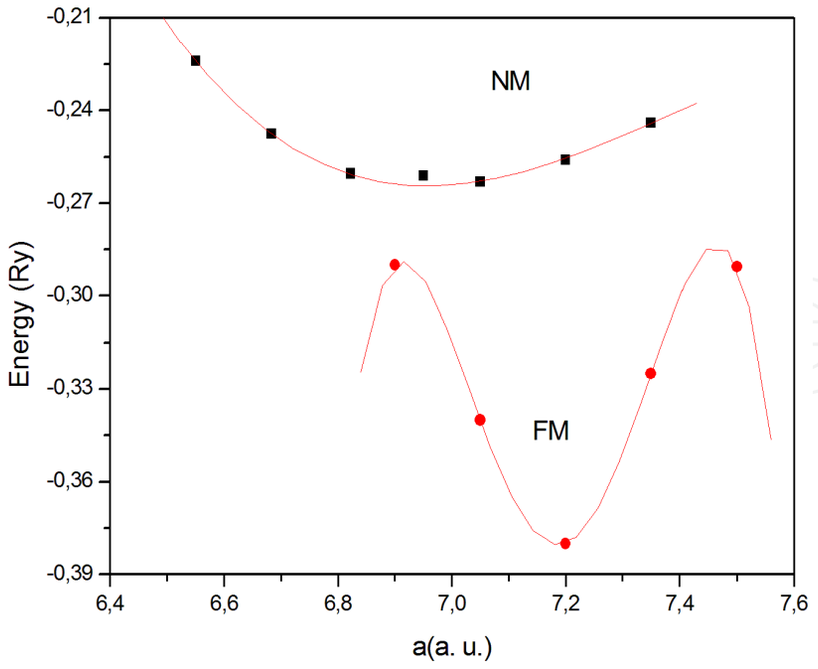


Figure 1. Total energy as a function of lattice parameters, the Fe / Pd bilayer. We did not present the error because they are smaller than the points.

agreement with the results in Table 1. The Fe-Pd interaction decreases the occupation of the d-down states in the ultrathin multilayers compared to the Fe-Pd and Fe nitrides 4PdN.

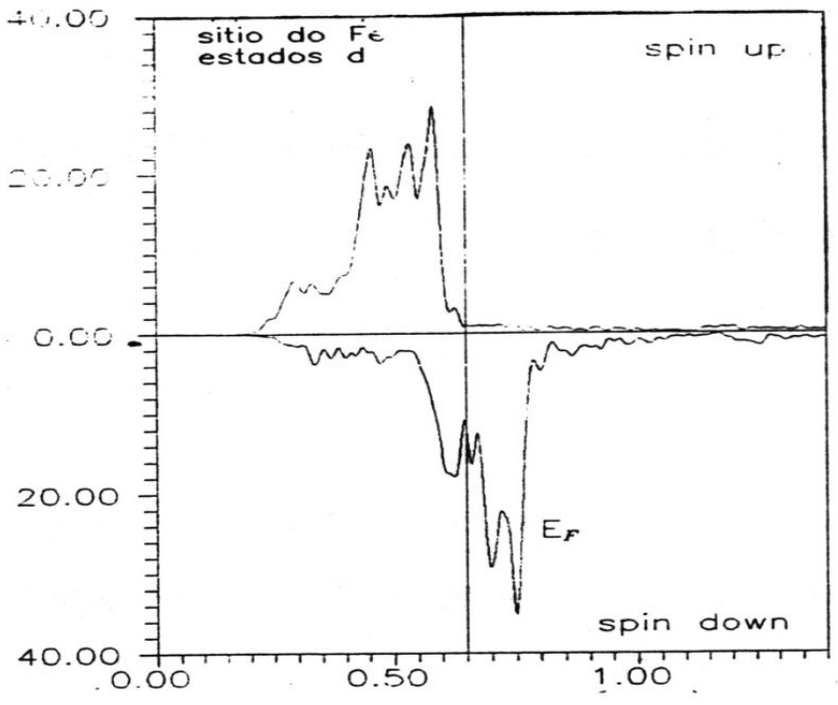


Figure 2. Density of states designed to electrons with spin up and down for d in the Fe / Pd bilayer in the Fe site.

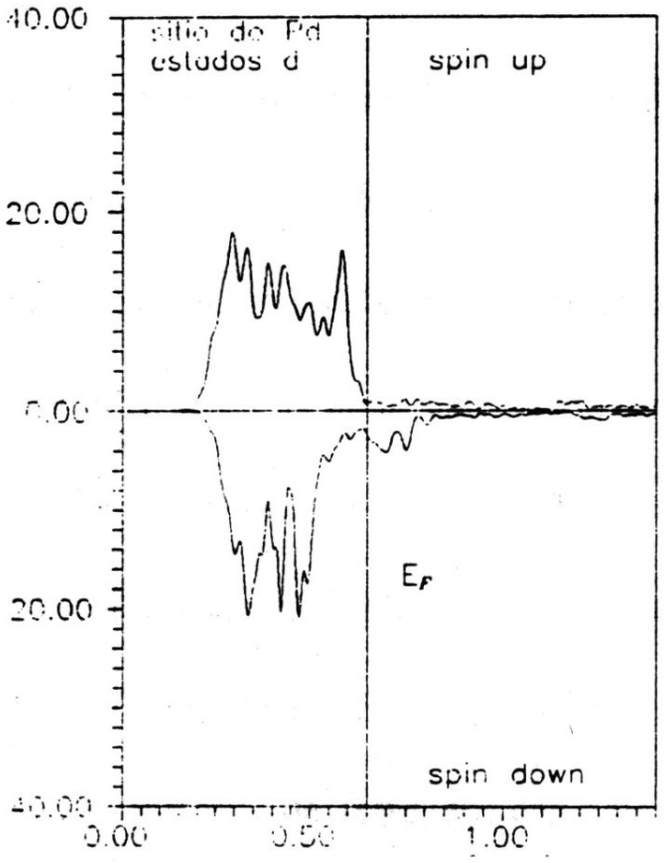


Figure 3. Density of states designed to electrons with spin up and down states for d in the Fe / Pd bilayer in the Pd site.

5. Pressure influence on the magnetic properties of the Fe/Pd ultrathin multilayers

Now, we investigate the behavior of the magnetic properties against pressure. The pressure effect is simulated by reducing the spacing of the lattice. We perform these self-consistent calculations for some lattice parameters of the Fe / Pd ultrathin multilayers, but we keep the tetragonal structure unchanged. The results of these calculations are shown in Figure 4. In this figure, we seethe variation of the magnetic moment on the site of the Fe and Pd due to the lattice parameter. In the Fe site, the magnetic moment decreases until the lattice parameter which sharply drops to zero. In the Pd site, the magnetic moment remains constant until it also falls abruptly to zero in the same lattice parameter a = 6,321ua. We can associate this lattice parameter limit value at a certain critical pressure. This type of behavior also happens in other leagues, known as Invar [56,57,60,61] alloys. Similar behavior of the magnetic moment has been obtained for iron carbides in ferromagnetic calculations [61]. We have published data from experimental studies on this fact in ultrathin multilayers of intermetallic materials systems.

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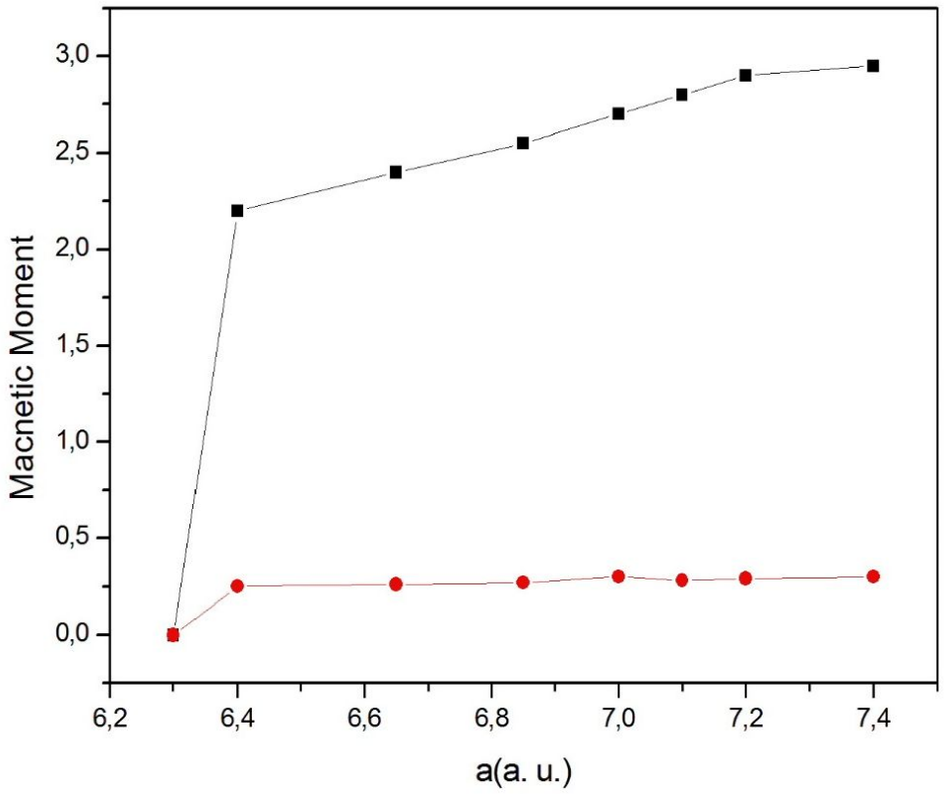


Figure 4. Magnetic moment due to the lattice parameter for the Fe / Pd, Fe, and Pd monolayers on site.

Fe				**Pd**		
	Up	**Down**	**Up-Down**	**Up i**	**Down**	**Up -Down**
n	4.1460	4.1459	0.0001	4.8537	4.8537	0.0000
n_s	0.3136	0.3136	0.0000	0.2841	0.2841	0.0000
n_p	0.4168	0.4168	0.0000	0.3672	0.3672	0.0000
N_d	3.4156	3.4155	0.0001	4.2024	4.2024	0.0000
$N(E_F)$	12.5957	12.6732		5.6340	6.6350	
$Nt(E_F)$		25.2689			11.2670	
$Nc(E_F)$			36.5359			
y			6.3320			
ΔQ		0.2921			-0.2921	
E_F			1.1399			

Table 2. Parameters calculated for spin polarization potential monolayers using self-consistent calculations. Here, n is in electron / spin; N in states / atom spin Ry; Nc states / Ry unit cell, y in mJ / molK2, EF Ry and ΔQ electrons. We obtain the critical pressure Pc = 109Kbar.

This result is of the order of the critical pressure of league ordered Fe-Pd [55], and also comparable to the theoretical and experimental results for Fe4Ni [59], Fe4PdN [57], and Fe_4SnN [60], which are made known to have the Invar behavior type and magnetic collapse with pressure feature. The issue of electronic redistribution due to this transition from the ferromagnetic state to the non-magnetic state will be discussed. To do so, we focus our attention in table 2, which shows some parameters obtained through the self-consistent calculation of the lattice parameter of the magnetic collapse shown in Figure 4. A comparison of Tables 1 and 2 show a large increase in the charge transfer to the site Fe. This excess charge will populate the state d spin down the Fe site, and also, there is an inversion of spin up electrons in the electron spin down that will cause the magnetic collapse. The results presented in Table 2 show that for high pressures, there is a redistribution. But this is not merely an average of the spin up and down, which existed before the occupation in Table 1. This redistribution is a consequence of the strong metal-metal interactions in front of the reduction of the lattice spacing. On the other hand, Table 2 shows an increase in the specific heat coefficient y. This value corresponds to a large number of states at the Fermi energy for the non-magnetic state. This growth occurs mainly in the up states, both in the Fe and the Pd sites.

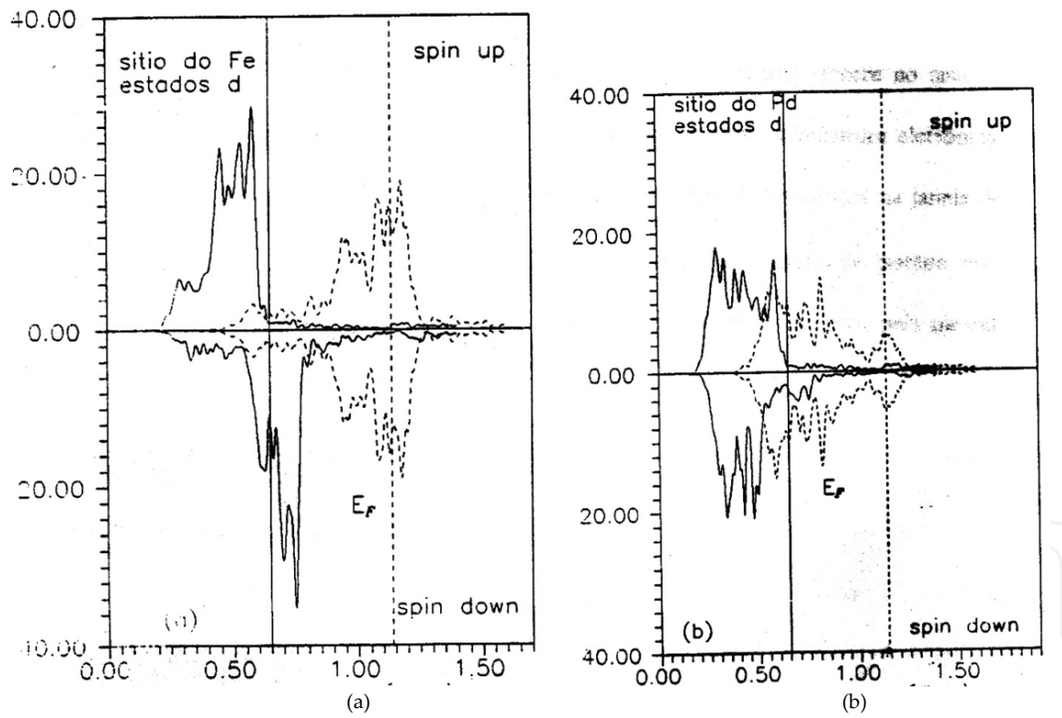


Figure 5. a -The DOS in the Fe site in the non-magnetic state (dotted lines) and in the ferromagnetic state (solid lines) are presented. b–The density of states designed for electrons with spin up and down states for d in the Fe / Pd bilayers: (a) at the Fe site in balance volume (solid lines), the magnetic collapse (dotted lines) and (b) Pd site in volume balance (solid lines), the magnetic collapse (dashed lines).

We noted that there was a widening of the band - d of the non-magnetic state in relation to the ferromagnetic state. Also, the DOS moves as a whole to higher energies, and the Fermi energy increases.

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In Figure 5b,we see the DOS in the non-magnetic (dashed lines) and ferromagnetic (solid line) states to the site of Pd. This site also promotes the DOS to a higher energy. Even in the magnetic collapse, some free states remain above the Fermi energy at the Fe site.

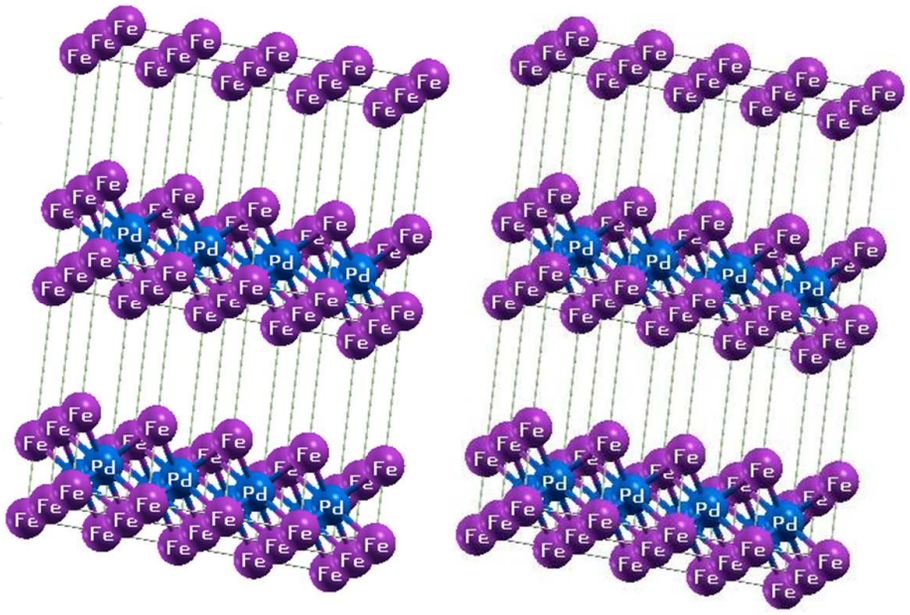


Figure 6. The unit cell of 2Fe / 2 Pd and Pd / Fe ultrathin multilayers.

6. The electronic structure of 2Fe/Pd and 2Pd/Fe ultrathin multilayers

In the rest of this chapter, we will study the 2 Fe/Pd and 2 Pd/Fe ultrathin multilayers. To accomplish the calculation of the band structure of the ultrathin multilayers of Fe-Pd, we introduced some modifications to the unit cell structure so we can have a better description of the actual physical system (1/2, 1/2, 0) for Pd and (0, 0, 0), (0, 1/2, 1/2) to the Fe atoms as bilayers in Figure 6. The structure used herein is a tetragonal structure of c / a = 2.23.

With this structure, we note that all Fe atoms have the same vicinity in the 2 Fe / Pd system. The above two systems used 1500 points in the power window and 1330 points k in the reciprocal space (we changed the number of points because we changed the crystal lattice). In the rest of this chapter, we will present the results of the calculations of the electronic structure and some comparisons between the systems. In the magnetic properties of the multilayer 2 Fe / Pd and 2 Pd / Fe, we performed the calculations of the total energy for some lattice parameters. With these calculations, we obtained the volume of theoretical equilibrium for both systems. Figure 7a shows the total energy states for the non-magnetic (NM) and ferromagnetic (FM) states of 2 Pd / Fe, depending on the lattice parameters. We used a three-degree polynomial to get the best fit curve. Figure 7b has the total energy as a function of the lattice parameter for the non-magnetic states (NM) and ferromagnetic (FM) states for the 2 Fe / Pd system.

We have noted that in both systems, there is a good stability of the ferromagnetic state in relation to the non-magnetic state. The energy of the difference in the volume balance between the ferromagnetic and non-magnetic state is ΔE = -13mRy by atom for the 2 Fe / Pd system. While in the 2 Pd / Fe system, the difference is even greater: ΔE = -20,7mRy by atom. Compared with the bilayer of Fe / Pd, we noted that they are more stable, since ΔE is even higher than the two systems: 2Fe / 2 Pd and Pd / Fe. These differences will be further explored when we discuss the influence of pressure on the magnetic properties.

The minimum total energy shows that the lattice parameter in the balance is 7,069ua for the ferromagnetic state and 6,890u.a for the non-magnetic state in the 2 Fe / Pd system. The lattice parameter for the ferromagnetic state was equal to 7,297uaand 7,209ua for the non-magnetic state. Thus, it is evident that if we put more layers of Pd, there will be an expansion of the Fe-Pd system, since the Pd atom is larger than the Fe atom. The magnetic moment calculated for the Fe site for both systems is high. We noted that the three systems studied in this chapter have magnetic moments on the site Fe, greater than the pure Fe, which is 2,217 μ_B. This is already known in the literature. Furthermore, this result agrees with the experimental [19] and theoretical studies performed by Richter et al. [29] to calculate the magnetic moment of Fe in place relative to the thickness of the multilayer. This suggests that increasing the number of Pd layers in the system increases the magnetic moment on the site Fe. Now, if we compare the magnetic moment on the Fe site with certain ordered alloys, we can note that it is larger and even greater than in nitrides [34,35,36,38,41]. In the Pd site, the magnetic moment has a different behavior from that found on the website of Fe, and the largest magnetic moment is in the 2 Fe / Pd system.

	Fe			**Pd**		
	Up	**Down**	**Up-Down**	**Up**	**Down i**	**Up-Down**
n	5.3700(5.5074)	2.6704(2.5247)	2.7096(2.9697)	5.1263(5.1523)	4.7863(4.8312)	0.3400(0.3211)
n_s	0.3268(0.3327)	0.3279(0.3327)	-0.00 11 (-.0043)	0.2834(0.2828)	0.2991(0.2949)	-O.OI57(-O.OI21)
n_p	0.3668(0.3676)	0.3756(0.3676)	-0.0088(-.0022)	0.3097(0.2995)	0.3291(0.2995)	-0.0194(-0.0091)
Nd	4.6864(4.8071)	1.9669(1.8309)	2.7195(2.9762)	4.5332(4.5700)	4.1581(1.5197)	0.3751(0.3423)
N(EF)	1.7855(1.2308)	12.6785(18.5056)		4.5332(4.9316)	1.9580(1.5197)	
N_T(EF)	14.4640(19.7364)			6.4913(6.4513)		
N_r(EF)				45.9223(27.3666)		
Y				7.9587(4.7428)		
E_F				0.6789(0.6109)		
ΔQ	0.0453(0.0351)			-0.0892(-0.0161)		

Table 3. Parameters calculated for the spin polarization in ultrathin multilayers volume balance of 2 Pd / Fe (in parentheses) and 2 Fe / Pd (outside the parentheses) using a self-consistent potential. Here, n is electron / spin; N in states / atom spin Ry; Nc states / Ry unit cell; y in mJ / molK2; EF Ry and ΔQ into electrons.

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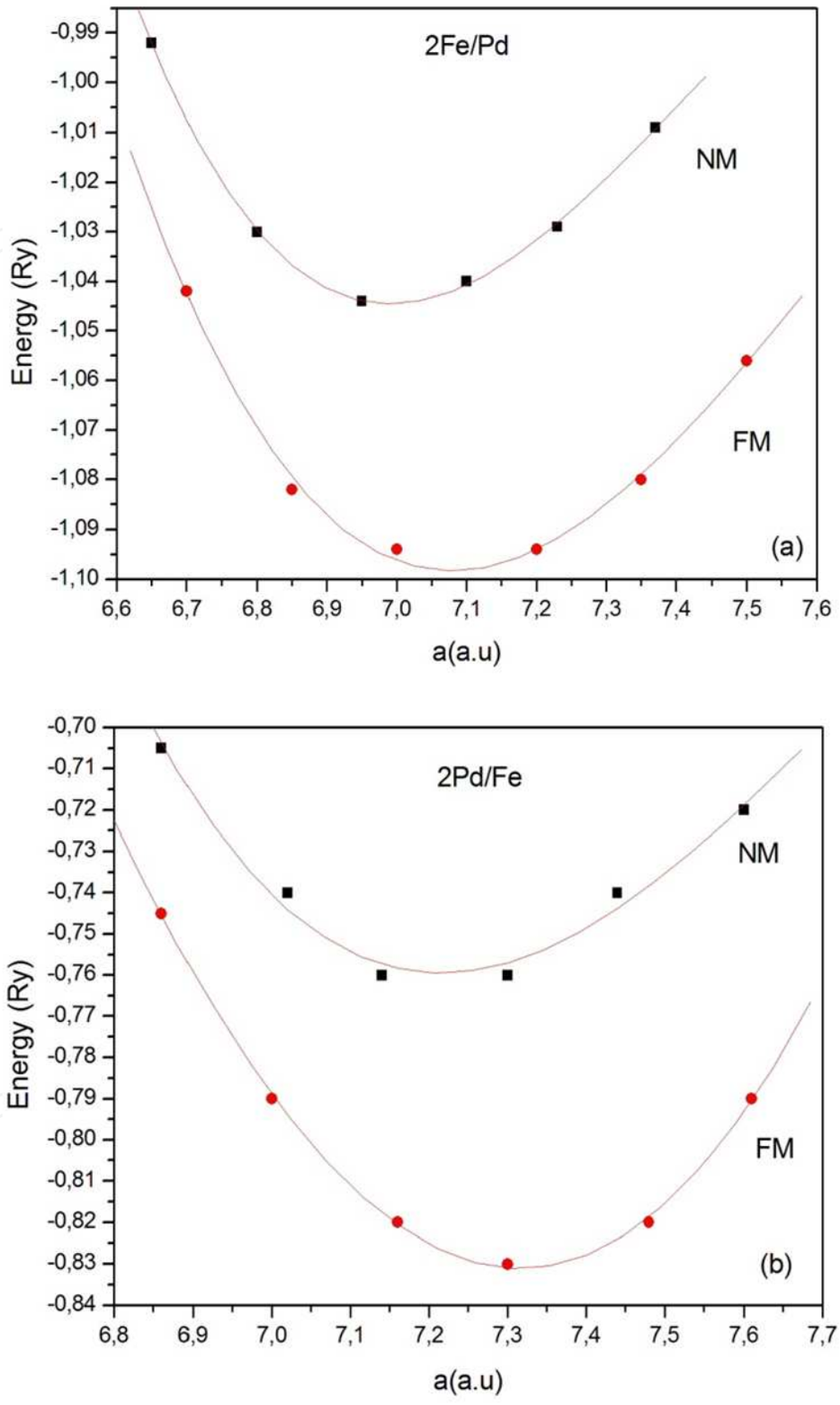


Figure 7. Total energy as a function of lattice parameters, the Fe / Pd bilayer. We did not present the error because they are smaller than the points. According to the energy parameter of the lattice ultrathin multilayers: (a) 2 Fe / Pd and (b) 2 Pd / Fe.

Table 3 -The specific heat coefficient, which is proportional to the total density of states and the Fermi level of the unit cell. We note that the 2Fe /Pd systems and 2 Pd / Fe is greater than that of the Fe / Pd bilayer where we now have a larger number of sites in the unit cell. The 2 Fe / Pd system is greater than 2 Pd / Fe, because the density of the states at the Fermi level is higher at the site of Fe in the Pd site. The Fermi energy is higher in the 2 Fe / Pd system. This shows that there is an increase in the Fermi energy when we increase the number of layers of Fe.

7. State density of the 2Fe/Pd and 2Pd/Fe ultrathin multilayers

The density of states for the electrons Fe and Pd multilayers are shown in Figures 8a, 8b, 9a, and 10b. Figures 8a and 8b show the DOS to the 2Fe / Pd system to the site of Fe (8a) and the site of Pd (8b) that spin in both directions, which is the balancing lattice parameter. In these figures, we noted initially that the Pd site states are all busy for both spin directions, but there are many empty down spin states in the Fe site. It is found in Figures 9a and 9b that DOS-d spin both directions of the equilibrium lattice parameter of the 2 Pd / Fe. In this system, we also found that for the Pd site, there are virtually no empty states above the Fermi energy, but in the Fe site, there are still several unoccupied states above the Fermi energy, as in the 2 Fe / Pd system.

Here, we find a change in the DOS form of a system to another. In the Pd site, there is a reversal peak height of up states in the 2 Pd/ Fe system with the next largest peaks at the Fermi energy. Also, a peak appears on the Pd site in the spin down states in the 2 Fe / Pd system where the area of energy is between 0,4Ry and 0,6Ry. This reflects the interaction with the states of Fe d down because if we look at the DOS on the Fe site in Figure 5.8a, we see that there is a peak in this energy range. Furthermore, this shows the influence of the two Fe sites on Pd since this interaction does not happen in the 2 Pd / Fe system.

8. Hyperfine parameters

It is evident that the Mossbauer Effect is an effective ferment when dealing with the magnetic structure of the nuclei and their interaction with the neighborhood. The hyperfine property related only to the site of the iron atom, the hyperfine field (in kg), and isomer shift (in mm / s) will be theoretically discussed. Initially, we propose that the magnetic field in the core is given by H = Hext + HFC + Horb + Hdip.

So, we understand that: Hext is the external applied magnetic field at the nucleus; and HFC is the hyperfine interaction (or Fermi contact term), which comes from an unbalanced spin density of the s-electrons can see these settings in references 30 and 31 with details.

To find the Fermi contact term we must use the following equation: gN is the nuclear gyro-magnetic ratio and y- (0) is the wave function at the nucleus for the spin-up and spin-down s-electrons.

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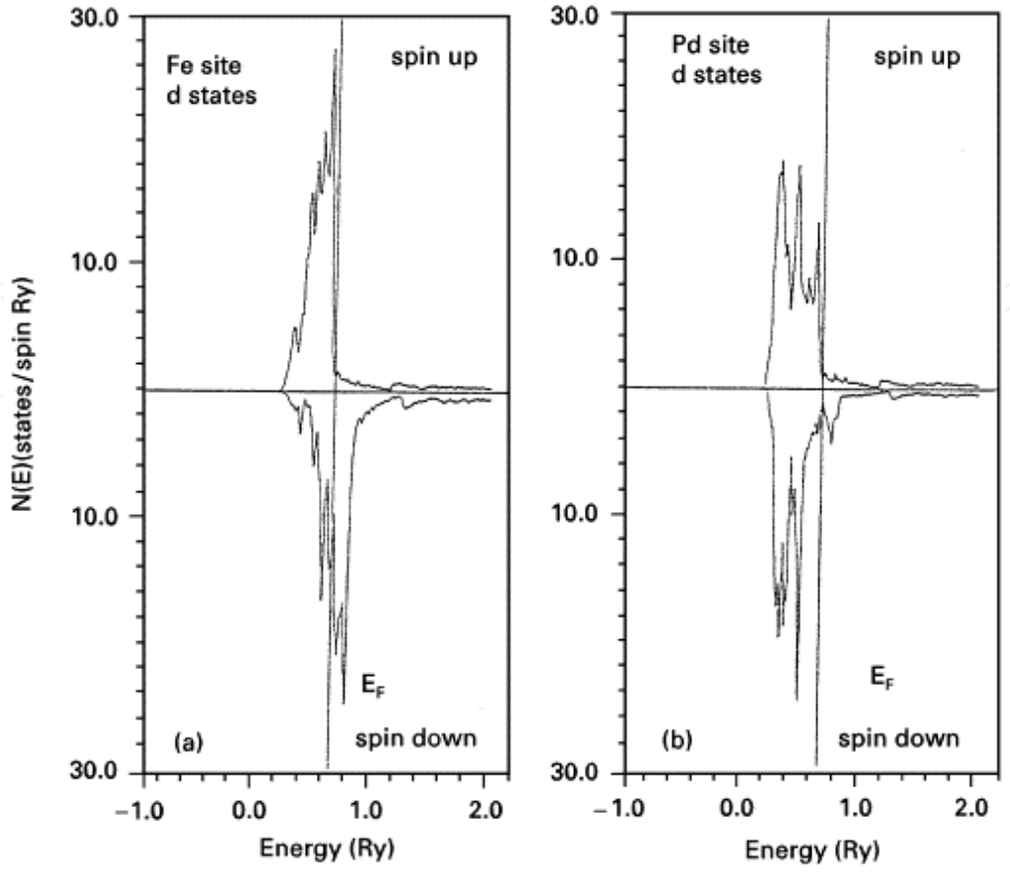


Figure 8. Density of states designed with spin up and down, to the states in d 2FePd / Pd ultrathin monolayers: (a) at the site of Fe and (b) the Pd site.

Another property to be calculated is the isomer shift of a given Beheerder atom comparing the nucleus electronic density ϱ (0) with a reference nuclei: α-Fe (BCC). In this case, Fe BCC with lattice parameters of a = 2865A °. Thus, the isomer shift is calculated by the Equation 6: where ϱa = Density of electrons in the nuclei; ϱs = Density of electrons in the reference nuclei; and α = constant of proportionality.

To understand the electron density in the nucleus, the isomer shift of a given atom is calculated comparing the nucleus electronic density ρ (0) with reference nuclei: α-Fe (BCC) in this case. The Fe BCC with lattice parameters of a=2865A°.Thus, the isomer shift is calculated by the Eq. 6: $IS = [\rho_a(0) - \rho_s(0)]\alpha$, where: ϱ_a = Density of electrons in the nuclei; ϱ_s = Density of electrons in the reference nuclei; andα = constant of proportionality.

In Table 4, we have the values of the HFC and IS systems for 2 Fe / Pd and 2 Pd / Fe. In this table, it is clear that if we change the neighborhood Fe site, there is a major change in the Fermi contact field. When we have2 Fe / Pd multilayer, we have the lowest Fermi contact term of the three systems, 210 kOe, which is less than the experimental value 330kOe of pure Fe. In the Fe bilayer / Pd multilayer and 2 Pd / Fe, we found the value higher than the experimental pure Fe. In the 2 Fe / Pd system, the site Fe receives loads of the Pd site, which will narrow the gap between the s electrons up and down causing a reduction in the Fermi contact field that is 210

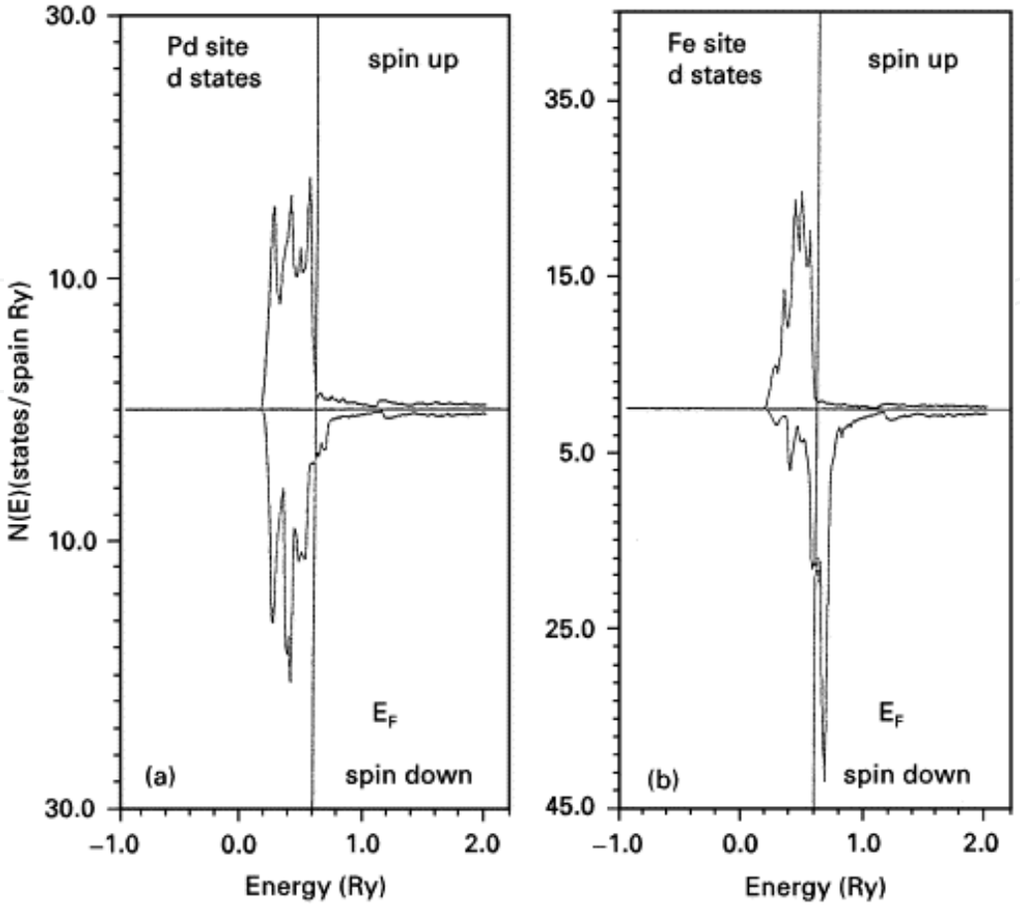


Figure 9. States density designed to electrons with spin up and down states for d in the 2 Pd / Fe multilayer: (a) the site Fe and (b) the Pd site.

kOe. When we have two layers of Pd, the charge transfer to the s states increases the difference between the electrons up and down, increasing the Fermi contact field (see table 4). This behavior of the Fermi contact field is consistent with the magnetic moment of the behavior on the site Fe, which confirms the empirical relationship of the magnetic moment that is proportional to the hyperfine field. Table 4 also shows the values calculated for the IS, which is greater for the bilayer Fe / Pd. The above results can be used for comparison with the experimental results of M. Li et al. [68,69], which show that when a Pd layer is placed in the 8Angstron, the Fermi contact field increased from 330 kOe to 335 kOe, which agrees qualitatively with our calculations. The differences are due to the calculations simulated at zero Kelvin temperature.

		H_{FC}(kOe)	IS(mm/s)
2Fe/Pd 2Pd/Fe	Fel	210	0.316
	Fe	388	0.456

Table 4. Hyperfine parameters calculated for 2 Pd / Fe and 2 Fe / Pd using spin polarization. Fermi contact term (HPC) in kOe, isomeric deviation (S) in mm / s.

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9. Influence of pressure on the magnetic properties and structure of the 2Fe/Pd and 2Pd / feelectronic ultrathin multilayers

In this section, we analyze the behavior of the magnetic properties and electronic structure of the 2 Fe / Pd and 2 Pd / Fe multilayer with pressure. We do this by varying the lattice parameter, which simulates a variation in pressure. Every self-consistent calculation submitted, the lattice parameter shows a variation of 2%. In Figures 10a and 10b, the magnetization shows as a function of the lattice parameter. Figure 10a shows the magnetization in the Fe site for both systems. We have noted that there is a different behavior between the two systems against the pressure. For the 2Fe / Pd system, there is an abrupt decrease in the magnetic moment of Fe, leading to the collapse of the magnetic moment. This transition from a ferromagnetic state to the non-magnetic state was obtained for the Fe / Pd bilayers [42].This behavior is observed experimentally in nitride [33] and in accordance with the calculations performed by bands [46]. In the case of 2 Pd / Fe, the pressure is not enough for a drop to zero in the magnetic moment. This behavior was observed in the alloys ordered Fe-Pd, depending on the Pd concentration in the league [34]. Figure 10b shows a similar behavior in the Pd site. However, in the 2 Fe / Pd system, there is a small increase of pressure in the magnetic moment in the Pd sites, but this is not very big. The 2 Pd / Fe system shows a different behavior: the magnetic moment does not drop to zero with increasing pressure and leaves a significant magnetization, as Fe-Pd alloys with the same proportions of Fe and Pd [32].

In figures 7a and 7b, we see the graph of the total energy as a function of the lattice parameter for the ferromagnetic and nonmagnetic states. From these data, we obtain the critical pressure of 92 kbar for the 2Fe / Pt system and 277 kbar for 2 Pd / Fe. Earlier in this chapter, we obtained a PC bilayer Fe / Pd with 109 kbar. It is clear that if we put more layers of Pd with respect to Fe, the PC system increases. These results are in the order of magnitude of ordered alloys Fe3Pd [34] and results to carbides Fe4C [42] and certain iron nitrides replaced [34,35,36,37,39]. In this situation, we noted that the multilayer has a similar behavior league that ordered the invar type.

Analyzing the decrease of the magnetic moment with increasing pressure, we studied the electron redistribution that occurred in the multilayer systems. Table 5 has some parameters obtained through self-consistent calculations for the spin polarization of the 2Fe / Pd systems (outside the parentheses) and 2 Pd / Fe (in the parentheses). Comparing Table 5 with Table 1, we noticed that there was an increase in the load transfer to the Fe site for both systems. This is due to the decrease of interatomic distances and the interpenetration of the electronic clouds. There was also a considerable increase in the density of states at the Fermi level for both compounds, which causes an increase in the specific heat coefficient y. The more general point is that there was an electronic redistribution in both systems. In the 2 Fe / Pd system, the transferred load Pd site to the Fe site population almost exclusively, the states d-down, together with a reversal of spin up electrons down, makes the non-magnetic system. Therefore, despite the pressure, the 2 Pd / Fe ferromagnetic state remains.

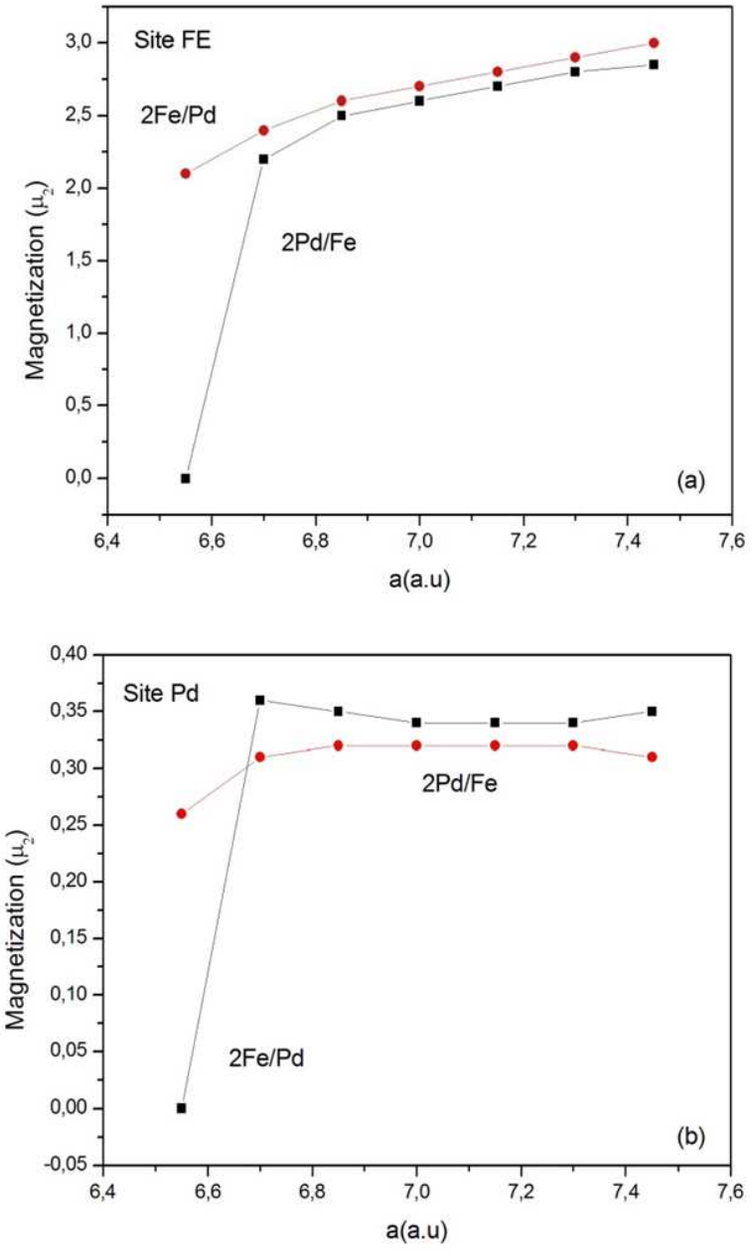


Figure 10. Magnetic moment due to the lattice parameter for ultrathin multilayers: (a) at the site of Fe and (b) Pd site.

Table 5 shows high pressure and low volume. And there is an electronics redistribution of the s electrons and this redistribution is not purely an average spin-up and down.

Figures 11a-d present the DOS for the spin-up and spin-down of the Fe site for both systems. In water, 6.5120 parameters with dotted lines for the2Fe / Pd system are shown, and full lines are seen for the 2 Pd / Fe system. We also noted that the d-DOS, as a whole, is moved to higher energies for both systems, but the 2 Pd / Fe d-DOS system is still taken to higher energies. There is also an increase in the Fermi energy of the system. It is clear that the 2 Fe / Pd system undergoes a transformation from the ferromagnetic phase to the non-magnetic phase, as in

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this system, there is practically no more difference between the area below the Fermi energy of up situations for the down states. In the Fe site of the 2 Pd/ Fe system, there is a difference between these areas that features a magnetic moment in this site.

The results shown in Figures 12 and 13 show a strong dependence of the HFC and IS with the spacing of the lattice, which is also checked for nitrides experimentally [33]. In all cases, the absolute value of the pressure decreases with HFC. This may be associated with the reduction in the contribution of the s electrons to the spin density at the core of Fe. We noted that for the 2Fe / Pd system in low volume. In the 2 Pd / Fe system with pressure, there was a decrease to zero for the HFC, and the same happens with the magnetic moment of the Fe site in this system (Figure 10). This confirms the proportionality between the HFC and magnetic moment. The IS behavior on the Fe sites due to the reduction in lattice spacing is quite similar for both the 2 Pd / Fe as well as for the 2Fe / Pd system. These results suggest that the difference between the hyperfine parameters can be related to the expansion of the lattice due to the larger radius of the atomic Pd atoms. In fact, the reduction in HFC when a Pd atom is replaced by the Fe atoms (2 Pd / Fe and 2 Fe / Pd) can be viewed as a simulation of applying pressure in the 2 Pd / Fe system (Figure 12).

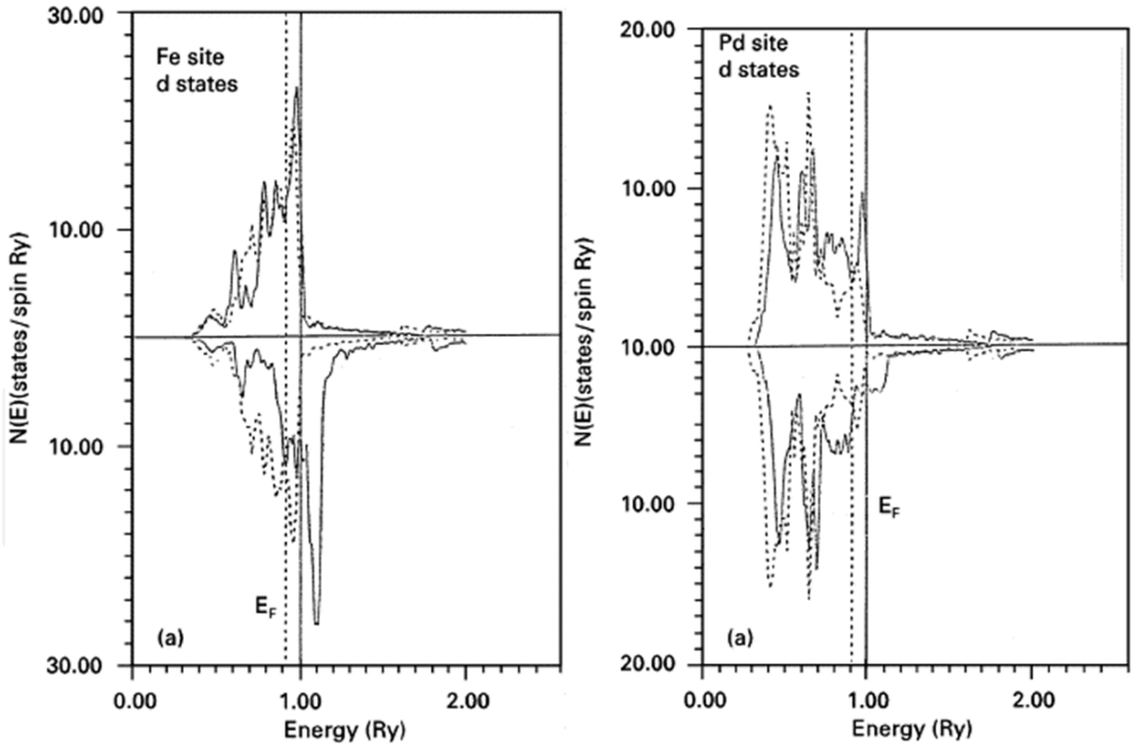


Figure 11. States that the density is designed to the electrons with spin up and down states for d, the multilayer 2 Fe / Pd, and 2 Pd / Fe. The volume of the magnetic breakdown are as follows: (a) the Fe site (solid lines 2 Pd / Fe), (dotted lines 2 Fe / Pd).

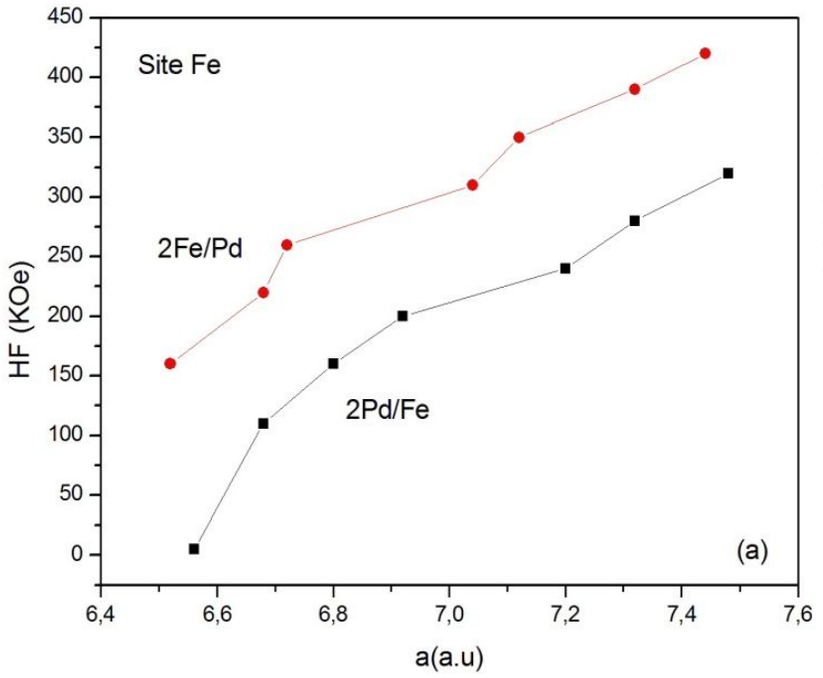


Figure 12. Hyperfine fields due to the lattice parameter.

10. Conclusion

In this paper, we used the LMTO method to the nearest ASA to investigate the electronic structure of ultrathin alloys, and the electronic structure of multilayer was analyzed.

The self-consistent calculations performed for the Fe / Pd ultrathin multilayers show a difference in the electronic structure when the stoichiometry of the multilayer systems is changed. As we increase the number of Pd layers relative to Fe, there is an increase in the magnetic moment on the website of Fe as well as an increase in the volume of the unit cell. Comparing the magnetic moment on the Fe site in the multilayer Fe / Pd alloys with certain ordered FePd and nitrides [32,33,39,40], we noticed a considerable increase. The hyperfine properties calculated for the multilayer Fe / Pd compared with the experimental results of M. Li et al. [42,43] have reasonable results from a qualitative point of view. The differences are due to the structure of the experimental multilayer, which is not ideal.

When subjected to pressure, the 2 Fe / Pd systems (2 Pd/ Fe and Fe / Pd) presented different behaviors among themselves. The 2Fe / Pd and Fe / Pd systems exhibited a magnetic collapse with an increasing pressure, while the 2 Pd / Fe magnetic moment were maintained in both the Fe and Pd sites. The hyperfine properties also changed with pressure.

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