First principle calculation of Fe and Fe(1)/Fe(5)/Fe(1) Slab bcc DOS and band structure

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In this paper we consider to the band structure analysis and calculated exact number of density of states with VASP simulation approximation to Kohn-Sham equation. As main conclusion which we expected and got from the calculation for the system is simple structure without any SOC or external strong magnetic field, will never take such a big fluctation which can affect the magnetic properties of the simple Fe-bcc and layer system.

Keywords: *First principle ınvestigation, simulation, electronic properties*

BACKGROUND

In the First principle calculation of the electronic structure usually starts from difficulties of many body Schredinger equation which is can be described by following hamiltonian of the system (Born and Oppenheimer, 1927; Hartree, 1928).

$$H = \sum_{i=1}^{N} \frac{1}{2}\nabla^2 + \sum_{i \neq j}^{N} \frac{1}{r_i - r_j} + U_{ext} \quad (1)$$

Here we have the Hamiltonian for many electron system under external field of nuclei in the system. Because of the very slow motion of nuclei we already assumed that system obey the Oppenheimer approximation. But w hen we are going to solve the Schredinger equation for many particle system wave function there is only possibility is numerical method.

That is why it is always good to separate of wave function onto-one map (Jones and Gunnarsson, 1989).

$$H\psi = E\psi$$
$$\psi = \prod_{i=1}^{N} \psi_i \quad (2)$$

Total energy of the system is a functional of density which is computed using the one-electron orbitals

$$\rho = \sum_{i=1}^{N} \psi^2_i(\vec{r}) \quad (3)$$

After this assumption one-electron orbitals are the solutions of the Kohn-Sham equation (Kohn and Sham, 1965).

$$\left(\frac{1}{2}\Delta + \Delta_Z + V_{Hartree} + V_{XC}\right)\psi_i = \varepsilon\psi_i \quad (4)$$

Here we have two important problem. First is the equation of motion for evolution of the system wave function is non linear differential equation (Zakharov and Manakov, 1974). Second originally comes from definition of charge density in equation (3). In fact second problem contains the circular problem i.e self consistency (Bickers, 2004).

Based on this background we are going to solve the density of states problem and band structure of Fe –bcc system and then consider the effect of perpendicular anisotropic magnetic effect.

Density of states and band structure of Fe - bcc

For calculation of the Fe-bcc DOS we need first of all to make a relaxation and to consider possible changes of the crystal structure of the system. In order to the basis data for calculation one way of possible VASP code is following in the first step for runnig relaxation of the system we need 4 input files which are

INCAR, KPOINTS, POSCAR and POTCAR. Indeed POTCAR usually given by the VASP itself. But other three input files should be created by users VASP (Vienna Ab Initio Simulation Package, 2022).

In our case for up and down spin distribution the result of simulation gives the following (Figure 1) distribution for DOS of simple Fe-bcc.

This result was expecting in order to the theory since, in the normal case Fe lattice structure is corresponds to bcc hence this is expected result.

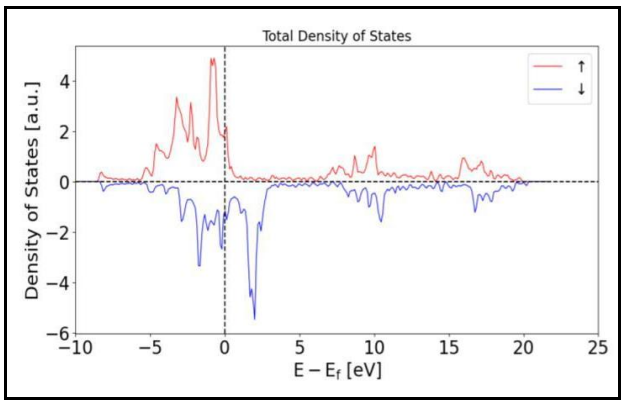

Fig. 1. DOS Distribution Fe-bcc.

For understanding the deep statement of the DOS distribution for the system Fe(1) /Fe (5)/ Fe (1). We have to emphasize the SOC between boundary layers of the system and because of the this arrangement we have the result below in figure 3 and 4. With small but main-important changes of inputs we we have this result.

If compare the two results, then it become clear there is a motion DOF of Slab case are seriously restricted and it is because of the interaction boundary electron clouds.

Other interesting thing here the band structure compration according to this results of DOS.

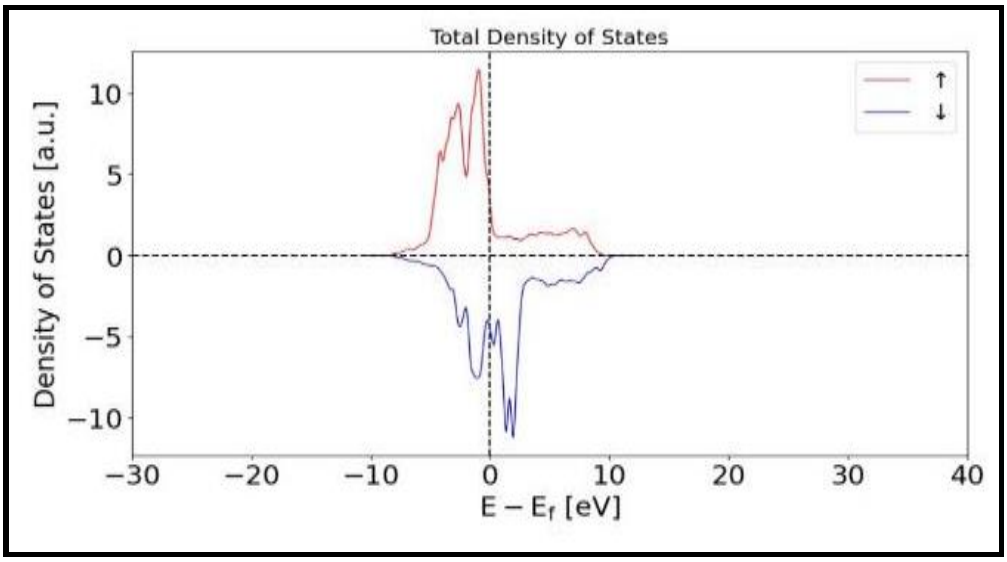

Fig. 2. Integral Total DOS distribution Fe-bcc.

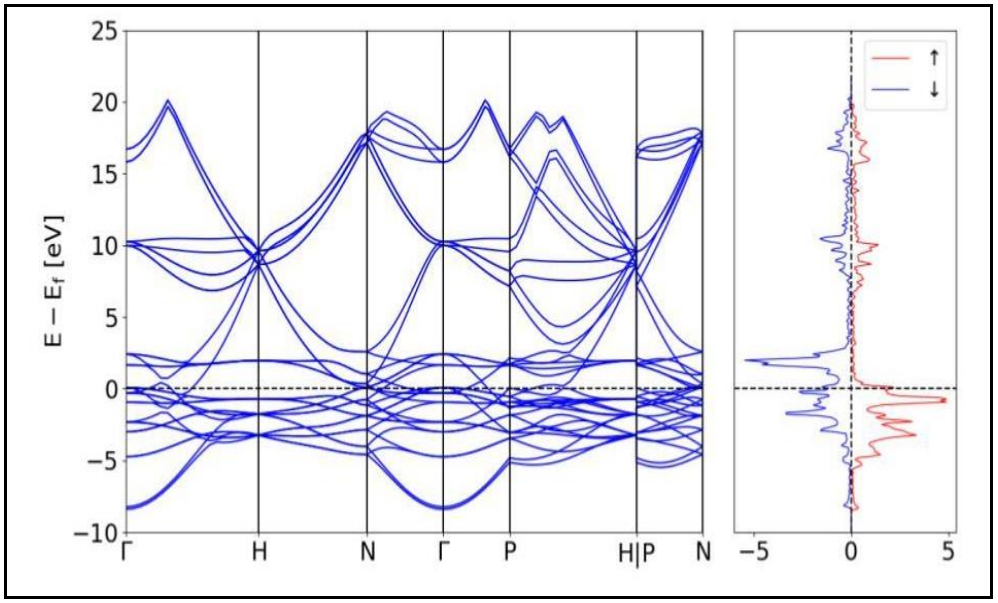

Fig. 3. Integral DOS file for Fe(1)/Fe(5)/Fe(1).

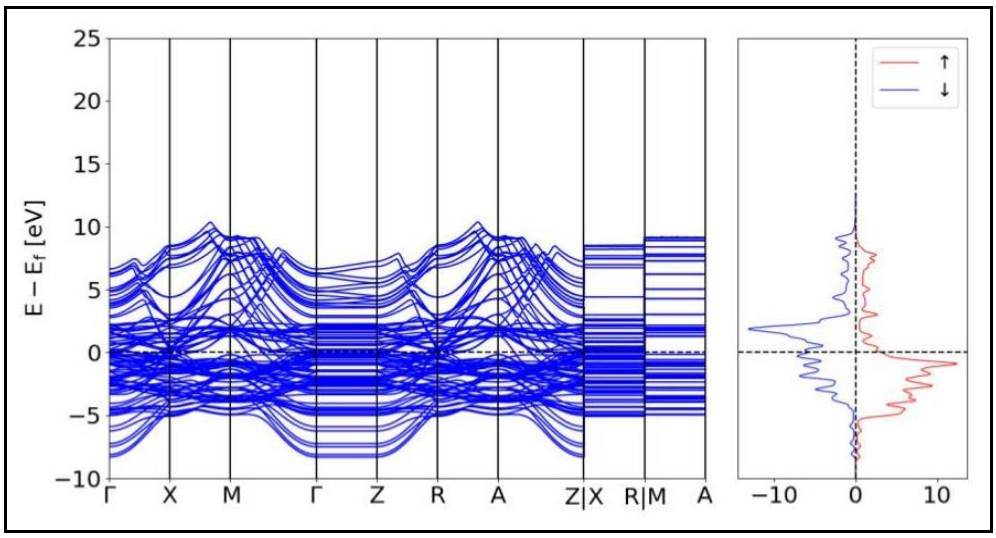

Fig. 4. Band Structure Density of States for Fe(1)/Fe(5)/Fe(1).

Here The electronic structure of the ideal of Fe slab has been calculated using the full potential linearized augmented plane waves (LAPW) technique in VASP Simulation package. Immediately compration the results with possible datas from literature have the following graph. From here it is very clear the difference of properties of s, p, and d orbitals.

CONCLUSION

As a conclusion it is obvious from both electronic properties (electronic density of states, band structure) says that however in the simple bcc case the DOF of last electrons are more than slab there is a slab case gives much more magnetic properties which can be converted to the industrial side of Magnetoresistance, MRAM mechanism and so on (Binasch et al., 1989; Tang and Pai, 2021). It is also interesting thing to get an investigation absolutely the same system but in different simulation packcege and to look is there any hidden difference between results. The same time still not so clear what will happen in the same type of system but under varying temprature dependence and dynamical movement of the system itself.

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Fe və Fe(1)/Fe(5)/Fe(1) Slab bcc DOS və əlaqə strukturunun birinci prinsip ilə hesablanması

Qarayev Güman Bəxtiyar oğlu

Azərbaycan Respublikası Elm və Təhsil Nazirliyi Molekulyar Biologiya və Biotexnologiyalar İnstitutunun Hesablama struktur biologiyası beynəlxalq laboratoriyası , Bakı, Azərbaycan

Məqalədə zolaq strukturunun təhlilinə və Kohn-Şam tənliyinə VASP simulyasiyasının yaxınlaşması ilə Hallarım sıxlığının dəqiq sayına diqqət yönəldilmişdir. Sistem üçün gözlədiyimiz və hesablamadan əldə etdiyimiz əsas nəticə ondan ibarətdir ki, heç bir SOC və ya xarici güclü maqnit sahəsi olmayan sadə quruluşlarda heç vaxt sadə Fe-bcc və təbəqə sisteminin maqnit xüsusiyyətlərinə təsir göstərə biləcək böyük dalğalanmalara məruz qalınmır.

Açar sözlər: *Birinci prinsip yaxınlaşması, simulyasiya, elektronik xususiyyətlər*