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RELATION ENTRE LA STRUCTURE ÉLECTRONIQUE ET LES  
 MODES DE GLISSEMENT DANS LES MÉTAUX DE STRUCTURE  
 HEXAGONALE COMPACTE

PAR

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RESUME

Tous les métaux de structure hexagonale compacte (HC) se déforment par glissement sur un système primaire (SPG) et plusieurs systèmes secondaires. Jusqu'à ce jour il n'existait aucun critère permettant de rendre compte ou de prévoir le choix du système primaire. Nous montrons dans notre communication qu'il existe une relation entre le système primaire de glissement (SPG) et la structure électronique de chaque métal HC. Nous avons calculé les énergies de faute dans le plan de base (EFB) et dans le plan prismatique (EFP) pour les métaux HC normaux (HCN), et les métaux HC de transition (HCT). Pour les HCN le calcul a été fait en utilisant les pseudopotentiels et pour les HCT en utilisant un modèle de liaison forte. Nous avons obtenu le résultat important suivant : EFP est toujours plus faible que EFB pour Ti, Y, Zr, Hf, Ru et Os; alors que pour Co et tous les HCN c'est EFB qui est plus faible que EFP; on propose alors que le rapport  $C_{44} \text{ EFP} / C_{66} \text{ EFB}$  pourrait être le paramètre qui contrôle le glissement primaire.

le 2 Février 1983

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COMMUNICATION AU SYMPOSIUM "THE STRUCTURE AND PROPERTIES OF CRYSTAL  
DEFECTS" LIBLICE DU 13 AU 17 JUIN 1983

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RELATIONSHIP BETWEEN THE ELECTRONIC STRUCTURE AND THE GLIDE  
IN THE HEXAGONAL CLOSE PACKED METALS

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I - INTRODUCTION

In all hexagonal close-packed metals (HCP), deformation is performed by slip on a mean glide system (MGS) and on several secondary systems. The mean system is basal ( $(0001) \langle 11\bar{2}0 \rangle$ ) or prismatic ( $\{10\bar{1}0\} \langle 11\bar{2}0 \rangle$ ) /1/. There are no reliable predictions of the MGS choice. Two assumptions have usually been made to account for the experimental results. The first, based on the geometrical ratio  $c/a$ , failed to predict the behaviour of beryllium, and clearly cannot explain the observed difference between Mg and Re, which have about the same  $c/a$  ratio. In the second, assumed by Regnier and Dupouy /2/, the choice of glide would be controlled by the stacking fault energy (SFE) in basal and prismatic planes. These authors suggested the SFE could be controlled by the presence or absence of an allotropic transformation (HCP to FCC for basal SFE; HCP to BCC for prismatic SFE). There is no experimental confirmation of these assumptions.

In this paper we show the role played by the electronic structure on the choice of glide system in HCP metals. First let us recall the following points: (1) in divalent HCP metals (Be, Mg, Zn, Cd) the MGS is basal, (2) for thallium, which is trivalent, MGS is basal or prismatic (the CRSS for both planes is the same), (3) in HCP transition metals of group III.A and IV.A (Y, Ti, Zr, Hf) MGS is prismatic, (4) in transition metals of group VII.A and VIII.A studied so far, MGS is prismatic or basal for Re, prismatic for Ru, and basal for Co, (5) in HCP rare earth metals (Tb, Dy, Er) studied, MGS is always prismatic /3, 4/. In summary we can see that MGS is basal for all normal metals and is a function of the electron number in HCP transition metals.

By analogy of the behaviour of the dislocations in BCC metals, we can assume that the choice of the glide plane could be controlled by the form of the core of the  $b = 1/3 \langle 11\bar{2}0 \rangle$  screw dislocation. Before calculating the configuration of the dislocation core, we need to know the value of the SFE. Consequently we have calculated these different SFE's using appropriate total energy models, for different metals. Thus we used pseudopotentials (or empirical pair potentials) for normal metals, and a tight-binding model for transition metals. With the help of these models, we drew the  $\gamma$ -surface maps /5/ and these results are presented in the following sections.

II - ESTIMATION OF S.F.E. IN NORMAL METALS

The  $\gamma$ -surfaces for the basal plane and the prismatic plane were calculated using : (1) a Lennard-Jones potential truncated between fifth and sixth nearest-neighbour shells (LJ5) and between sixth and seventh nearest-neighbour shell (LJ6), which is considered to be appropriate for a simulation study of HCP metals /6, 7/, (2) ion-ion pseudopotentials for Be, Mg, Zn, Cd.

The important characteristics of the  $\gamma$ -surfaces are the following : the prismatic  $\gamma$ -surface (fig. 1a) does not possess any local minima, which means that no stable single layer stacking fault may be formed on (1010). However we can speak of a generalized splitting with unstable stacking fault. The Burgers vector of fractional dislocations will be continuously distributed in the fault and is parallel to the compact direction  $\langle 11\bar{2}0 \rangle$ . Let us call the mean value of this unstable fault,  $\gamma$  prismatic =  $1/2 [\gamma(.2b) + \gamma(.3b)]$ .

In the basal  $\gamma$ -surface there is a pronounced minimum in all cases for  $\vec{f} = 1/3 \langle 10\bar{1}0 \rangle$ , which is the well known  $\vec{f}$  vector of the stacking fault in the HCP metals (fig. 1b). The basal fault is always smaller than the prismatic one (by a factor 2 to 10). Therefore it is not surprising that Bacon and Martin /6/ cannot observe the prismatic slip as the primary slip, using the potentials LJ5 or LJ6. Our results account well the experimental fact that MGS is basal in all normal metals.

### III - ESTIMATION OF S.F.E. IN TRANSITION METALS AND CONCLUSION

To estimate the cohesive energy, we use the model from Ducastelle /8/ : E cohesion = E binding + E repulsive. E binding is the "d-bonding" energy, which we calculate with a tight-binding description of the d-band. The local density of states is derived either from the gaussian approximation /11/, or from the recursion method /9, 10/ with 9 pairs of coefficient. A common set of parameters is used for all metals :  $dd\sigma = -2S$ ,  $dd\pi = S$ ,  $ddS = 0$ ; S being a scaling factor to yield the real crystal bandwidth. E repulsive is a repulsive term arising from the compression of the sp electrons and is empirically represented by a Born-Mayer type interaction.

The basal SFE is an oscillating function of the "d-band" filling (fig. 2). The difference between our values and Papon et al's ones /11/ comes from the fact we take into account the second neighbour's integrals. Details of calculation will be published later /12/.

With the gaussian approximation, the  $\gamma$ -surface for the prismatic plane (fig. 3) has the same shape as that obtained with pair potentials. All the calculated values are in table I.

The most important results are the following : (1) prismatic SFE (PSFE) is smaller than basal SFE (BSFE) for Y, Ti, Zr, Hf, Ru and Os; (2) BSFE is smaller than PSFE for Co and all normal metals; (3) BSFE and PSFE are about the same for Re and Tc.

In conclusion, if we assume that the ratio  $R = C_{44} \times PSFE / C_{66} \times BSFE$  is the control parameter for glide, we find three domains (1)  $R > 1$  : basal glide, (2)  $R \approx 1$  : indifferent; (3)  $R < 1$  : prismatic glide. The experimental results are in excellent agreement with this assumption.

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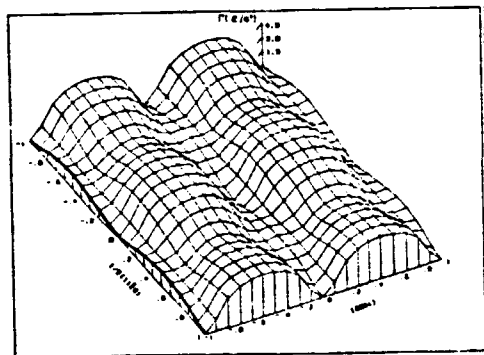


Fig. 1a : The (relaxed)  $\gamma$ -surface of the LJ6 crystal on (1100)

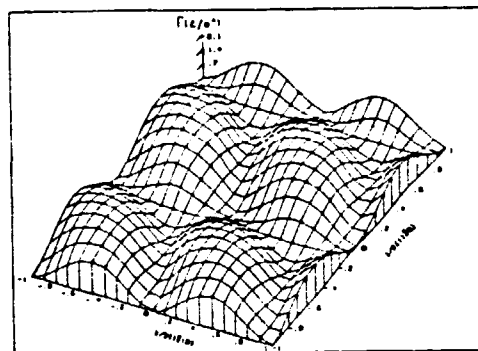


Fig. 1b : The (relaxed)  $\gamma$ -surface of the LJ6 crystal on (0001)

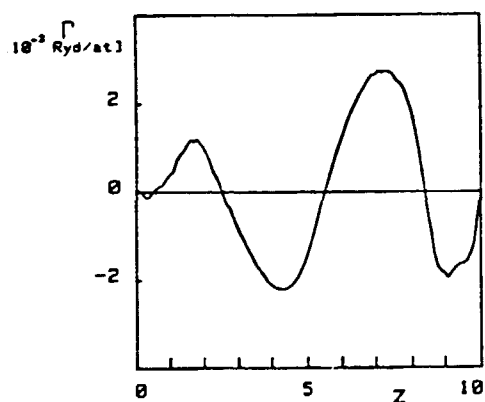


Fig. 2 : B.S.F.E. versus d-band filling in HCP structure

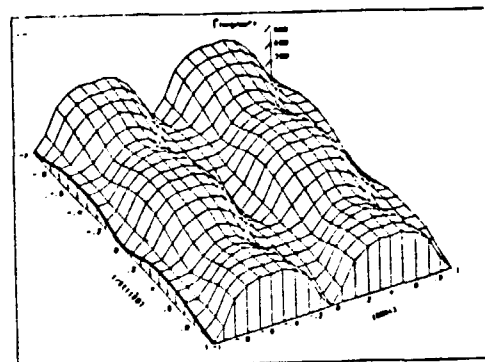


Fig. 3 : The (relaxed)  $\gamma$ -surface of Ti on (1100)

	Cd	Co	Mg	Zn	Be	Re	Tc	Ru	Os	Hf	Zr	Ti	Y
B.S.F.E.	15	45	30	35	390	540	470	875	1050	390	340	290	210
P.S.F.E.	150	230	125	210	620	680	440	520	600	185	150	110	60
R	.2	.2	.25	.25	.6	.9	1	1.7	1.8	2.1	2.3	2.6	3.5
M.G.S.	B	B	B	B	B	B/P	?	P	?	P	P	P	P

R < 1
R = 1
R > 1

Table I

