



INTERNATIONAL ATOMIC ENERGY AGENCY  
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION  
**INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS**  
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SMR/697  
7-Mag.Mult.

**RESEARCH WORKSHOP ON CONDENSED MATTER PHYSICS**  
(21 June - 3 September 1993)

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**WORKING GROUP ON MAGNETIC MULTILAYERS**  
(9 - 13 August 1993)

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**INTERFACIAL AND INTERLAYER MAGNETIC  
COUPLING IN METALLIC SUPERLATTICES**

**PART I**

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**These are preliminary lecture notes, intended only for distribution to  
participants**

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# INTERLAYER MAGNETIC COUPLINGS

## IN METALLIC SUPERLATTICES

- a brief survey -
- the theoretical understanding -

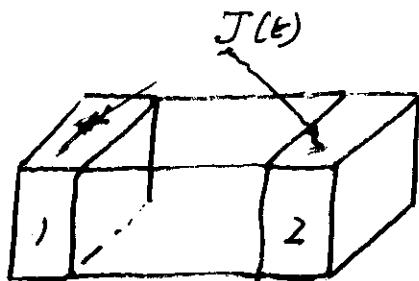
$A_m B_n$

A	B	
Fe, Co, Ni	Cu, Al Ru Ir	NM
	Pd	NFM
	Cr, Mn ...	AF
		F
FERRO LAYERS	SPACERS	

m, n      SOME MONOLAYERS

D. Scheffler, K. Oyaedela, J. Sticht, F.G.  
;

- MAGNETIC COUPLINGS



MAGNETIC ORDER

AF  
F  
KELI ?

$J(\epsilon)$  ?

• LONG RANGED

$$\Delta E = \frac{J^2}{2} \frac{M_1 M_2}{d} \cdot \frac{1}{\epsilon}$$

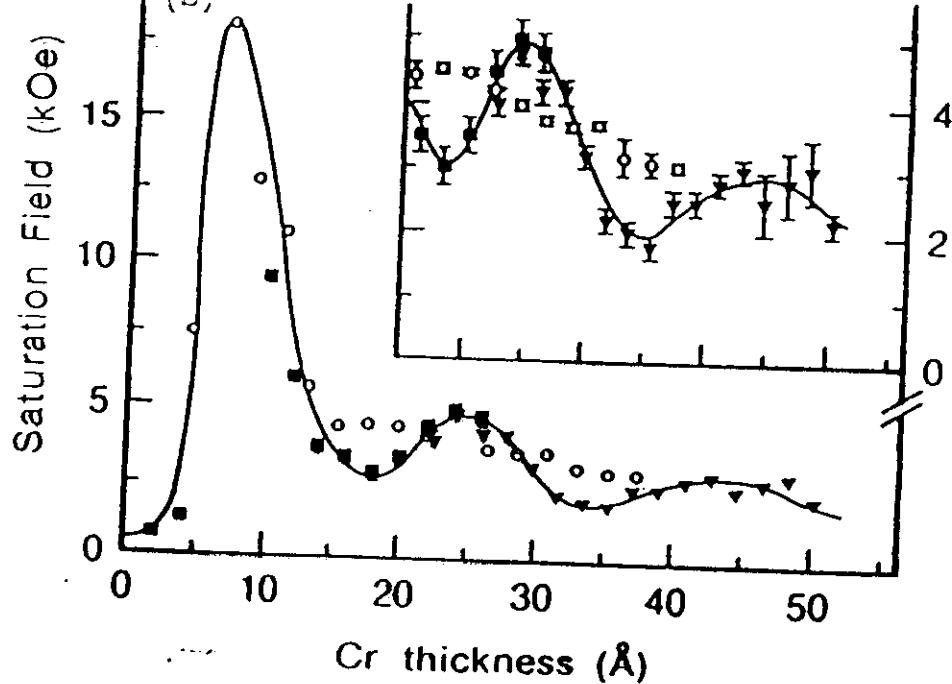
- OSCILLATING  $\sim 3 - 10 \text{ \AA}$  PERIOD
- DETERMINED BY THE SPACER (NH, N, AF...)
- DEPEND STRONGLY ON THE NATURE OF THE INTERFACES
- NECESSITY OF BETTER CONTROL OF THE QUALITY OF THE SL TO UNDERSTAND THE ORIGIN OF THE MAGNETIC SPLITTING

- AS AN EXAMPLE THE Cr-Fe SUPERLATT.

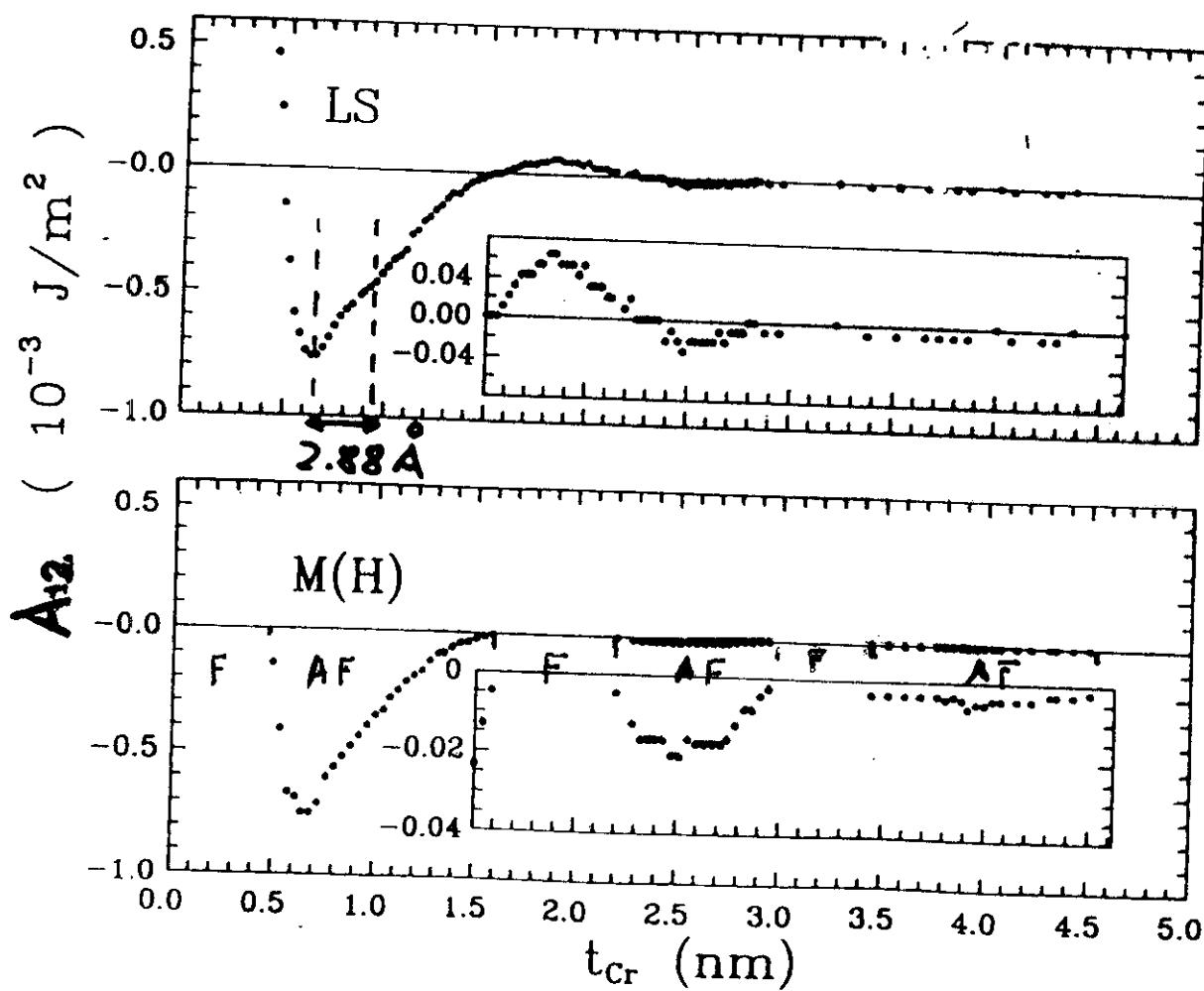
# Cr Fe SUPERLATTICES

- 1 AF COUPLINGS BY SPLEED AND BRILLOUIN  
Grunberg 1986 Carbone Alvarado 1987
- 2 AF COUPLINGS FOR  $m < 15$   
GIANT MAGNETORESISTANCE Baibich et al 1988
- 3 OSCILLATING COUPLINGS:
  - EXP LONG PERIOD ( $\sim 18 \text{ \AA}$ )  
Parkin 1990  
Grunberg 1991
  - THEORY SHORT PERIOD ( $\sim 4 \text{ \AA}$ )  
Stauffer F.G. 1990  
Hermann 1991
  - EXP : SYSTEMATICS FOR ALL TM SPACES  
Fe/A Parkin 1991
- 4 SHORT AND LONG RANGE OSCILLATIONS  
ACCORDING TO THE CRYSTALLINE QUALITY OF  
THE LAYERS (Mguris 91)  
 $(4 \text{ \AA}$  and  $10 \text{ \AA}$ )
- 5 Cr is AF AT HIGH TEMPERATURE:  
"AF SPACES" Mguris 92.

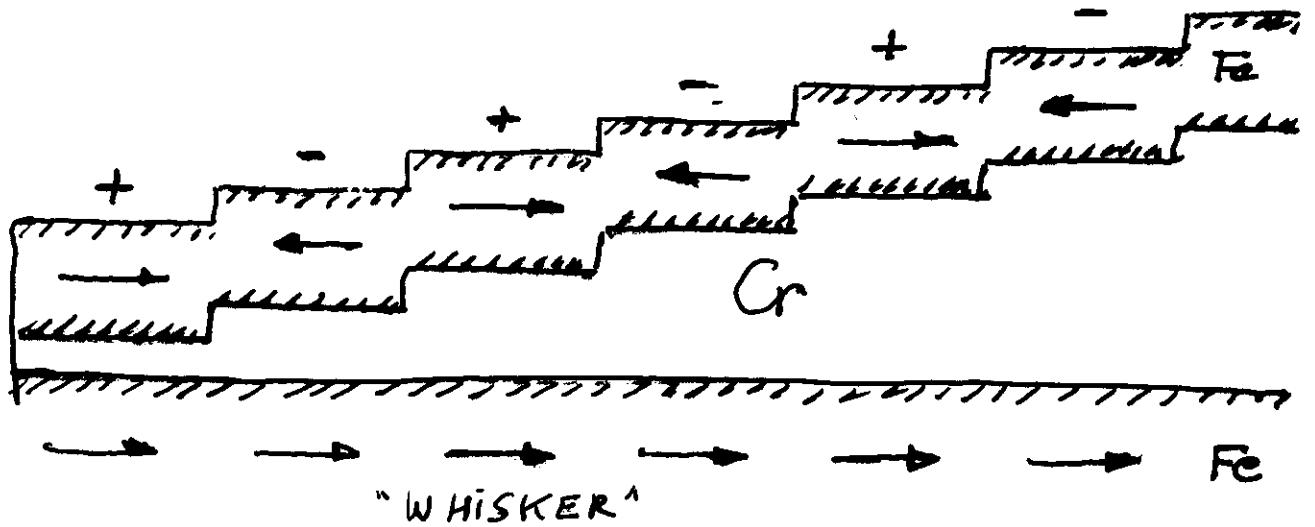
- A<sub>12</sub>.



saturation field (4.5 K) vs Cr layer thickness for three series of structures of the form Si(111)/(100 Å) Cr/[(20 Å) Fe/ $t_{Cr}$  Cr] $_N$ /(50 Å) Cr, deposited at temperatures of  $\Delta$ , ■, 40°C ( $N=30$ ); ○, 125°C ( $N=20$ ).



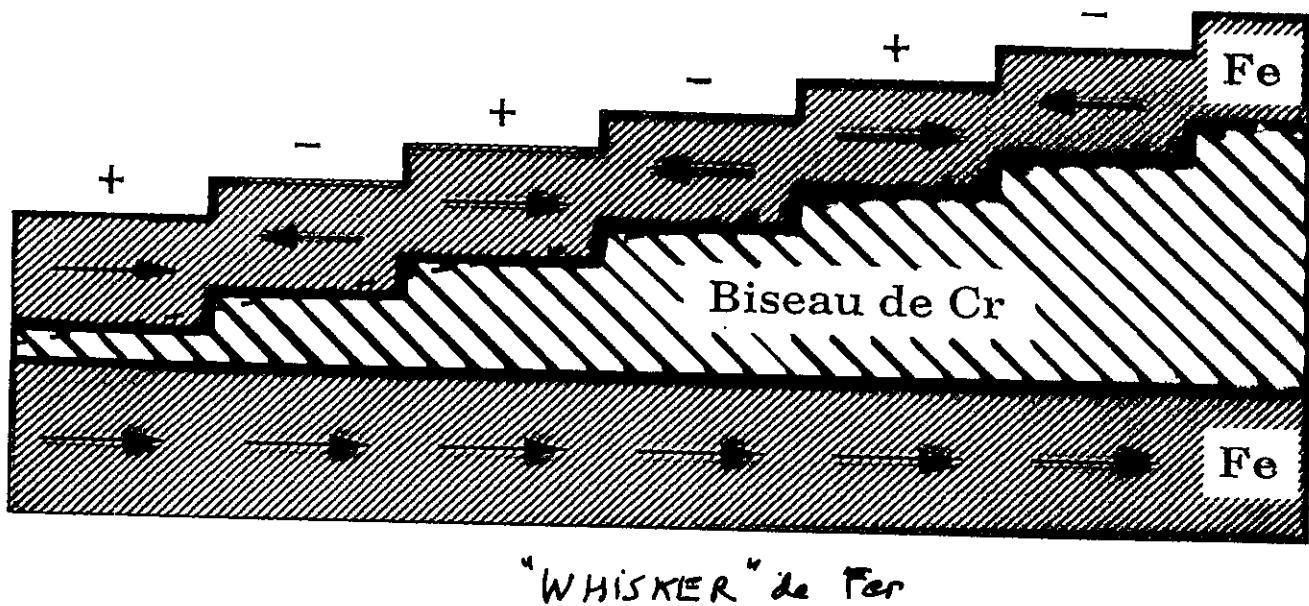
Grunberg et al 1992



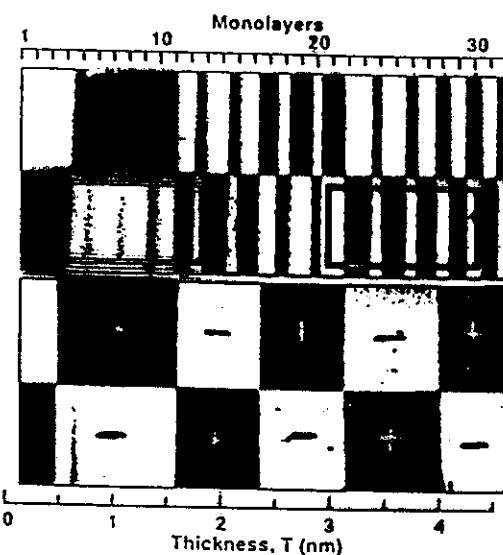
GOOD CRYSTALLINE QUALITY  $\rightarrow \Lambda \approx 2 \text{ MC}$   
 $\Lambda \times 9 \text{ MC}$

Ungun et al 1991

-Mise en évidence de deux périodes d'oscillation: rôle de la rugosité interfaciale (Ungar et al., 1991)



Bonne qualité  
cristalline à l'interface:  
COURTES PERIODES →



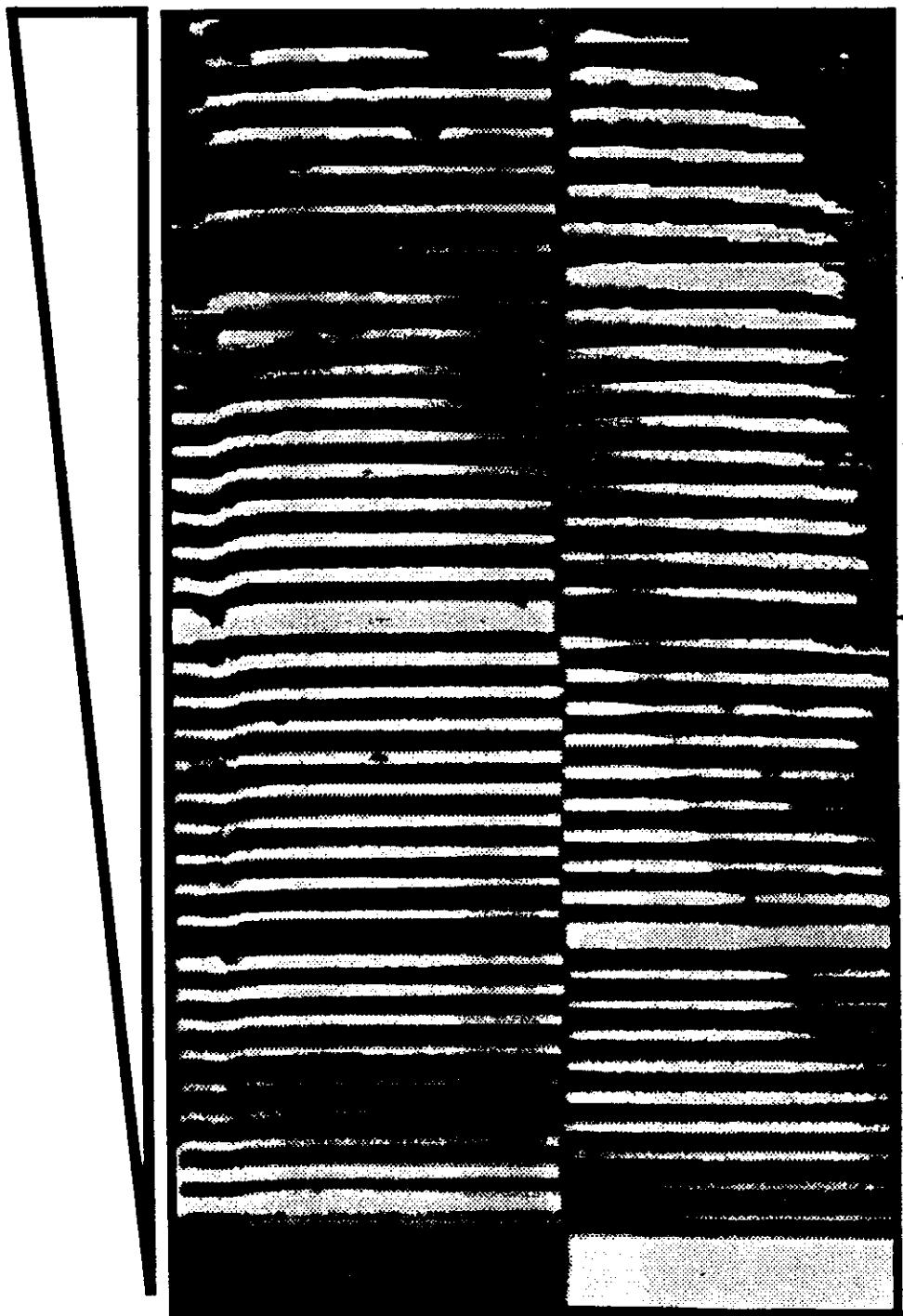
Moins bonne qualité  
cristalline à l'interface:  
LONGUES PERIODES →

Ungar et al 1992

- 3 -

SHORT AND LONG PERIODS !

.6

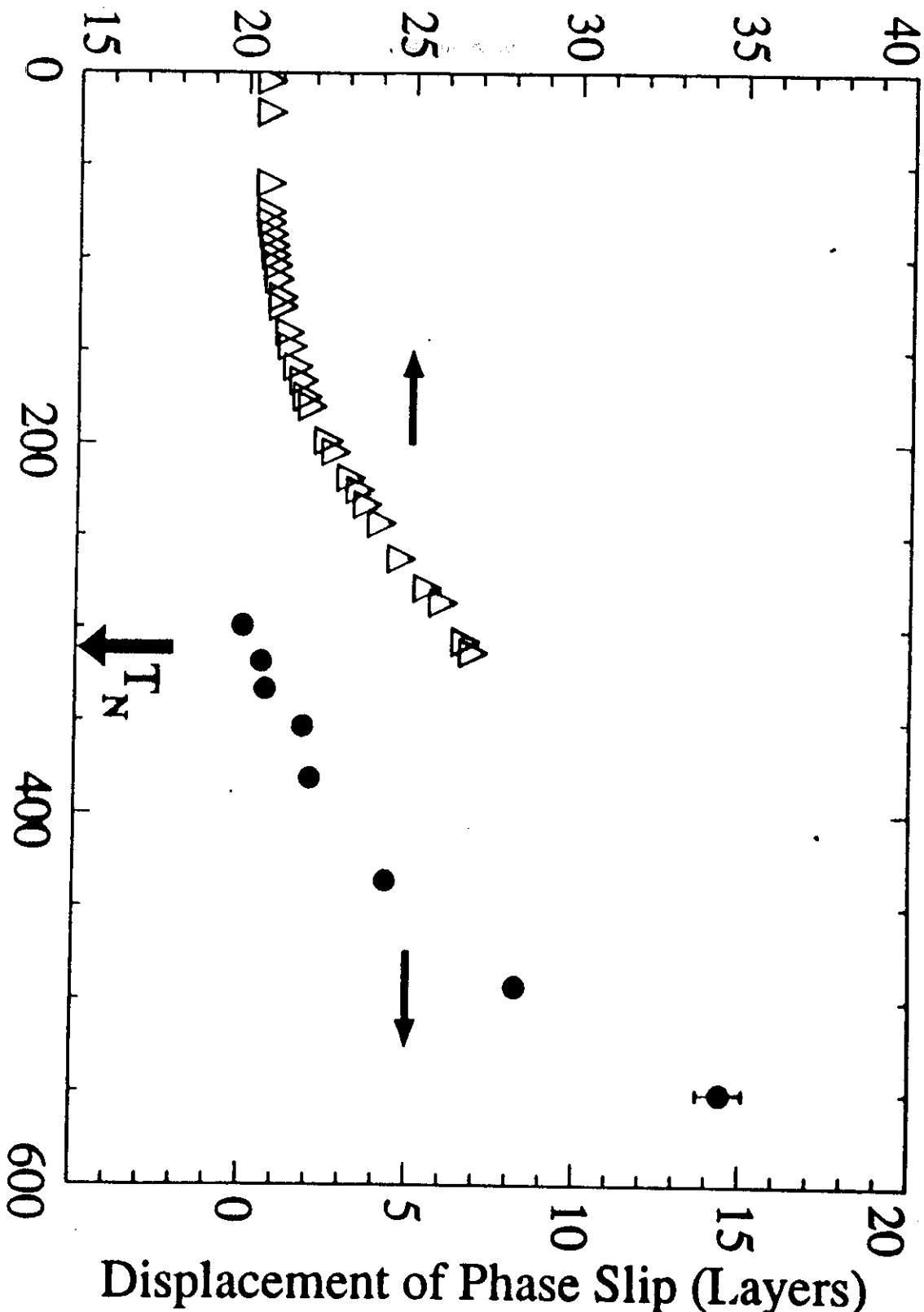


PHASE SLABS      1993

⇒ PHASE SLABS

Fig 1

# Distance Between Phase Slips (Layers)



# I. M. C

- 1 INTRODUCTION
- 2 INC : THE THEORETICAL SITUATION
- 3 CALCULATION OF THE INC - METHODS
- 4 1st EXAMPLE : THE Pd Fe SYSTEM
- 5 2d EXAMPLE : THE Cr Fe SYSTEM
  
- POINT OUT THE LIMITATIONS (and POSSIBILITIES  
OF THE METHODS)
- CONSIDER MOSTLY THE RESULTS OF BAND STRUCT  
CALCULATIONS

## 2 IMC : THEORETICAL SITUATION

### 2-1 "RKKY" MODELS

- |                 |             |      |
|-----------------|-------------|------|
| Yafet           | 1987        | Gd Y |
| Levy Wang       | 1990        |      |
| * Bruno Chapput | 1991 - 1993 |      |
| Edwards Mather  | 1990 - 1993 |      |

### 2-2 BAND STRUCTURE MODELS

#### • L.S.D.A.

- |                 |             |                     |
|-----------------|-------------|---------------------|
| Ongaydala et al | 1989 - 1991 | Fe Cr               |
| Koenig Knab     | 1991 - 1993 | Fe Ru               |
| Hermann Strubel | 1991 - 1993 | Fe Cr <del>Al</del> |
| Stoeffler et al | 1992 - 1993 | Co Ru, Pd I.        |

#### • TIGHT BINDING MODELS (TB)

- Stoeffler et al 1990 - 1993

### 2.3 LIMITATIONS

#### • RKKY

ASYMPTOTIC REGIME

$$\Delta > \Delta_1$$

+ SIMPLIFYING ASSUMPTION

#### • BAND STRUCTURE MODELS

SMALL  $\epsilon$  ( $\epsilon <$ )

"ab initio"

+ LSDA + STRUCTURE +

"TB"

+ SEMI-EMP PAR

### 3. DETERMINATION OF THE INTERLAYER COUPL.

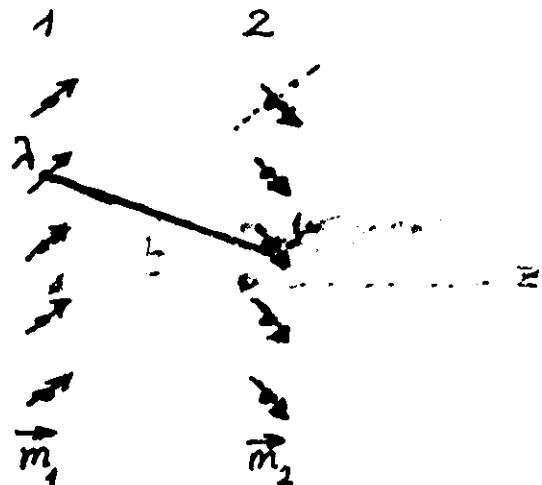
a)

#### INTERLAYER MAGNETIC COUPLINGS "RKKY"

- 2 FERRO. PLANES 1, 2 A

PERTURBING AN EL GAS B

(ex A = Cr, B = Cu)



- EACH IMPURITY A INTRODUCES

A PERTURBING POTENTIAL  $V_\alpha(r)$

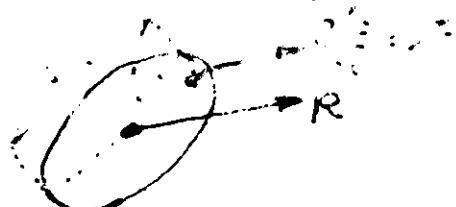
AND A SPIN POLARIZATION  $\vec{m}_\alpha(r)$

- THE INTERACTION ENERGY BETWEEN THE PLANES OF A RESULTS FROM THE SUPERPOSITION OF THE PAIR INTERACTION BETWEEN  $\lambda \in 1$  AND  $\mu \in 2$

"QUADRATIC EXCHANGE"  $E(E) = \sum_{\lambda, \mu} \delta(\lambda - \mu) \hat{\vec{m}}_\lambda \cdot \hat{\vec{m}}_\mu$

- ASYMPTOTIC FORM  $t \rightarrow \infty$  (The  $V_\alpha$  are assumed to be localized)

IMPURITY Blandin 1960  
 $R$   
 $r(\lambda - \mu) \sim \sum_\alpha A_\alpha \frac{c_0(D_\alpha R + q_\alpha)}{R^3}$



PLANES Bruno  
 $E(t) \sim \sum_\beta A_\beta \frac{c_0(D^\beta t + q^\beta)}{t^2}$



THE PERIOD OF THE IMC OSCILLATIONS DETERMINED BY  
THE TOPOLOGY OF THE FERRO SURFACE  
AMPLITUDE? PHASE? BIQUADRATIC?

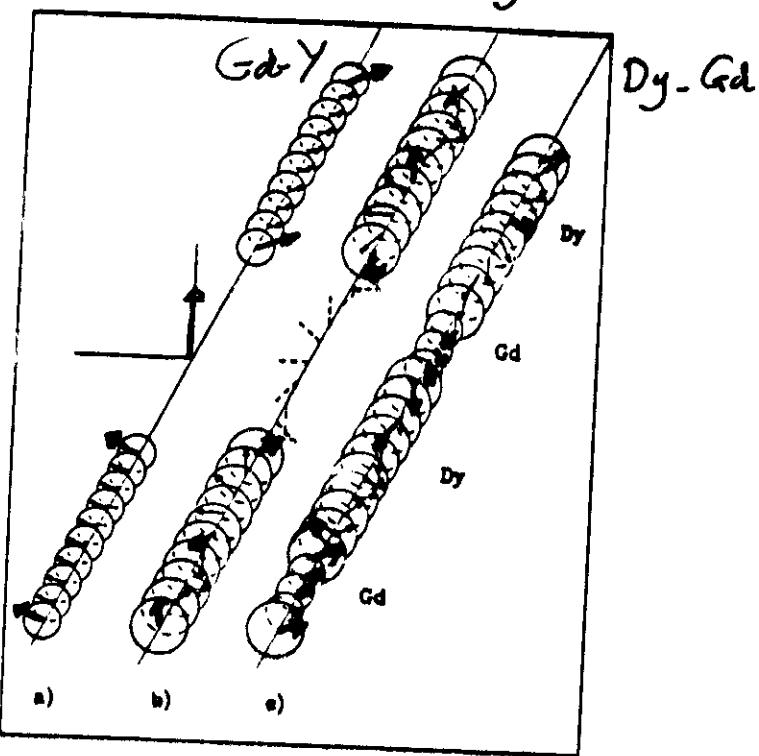
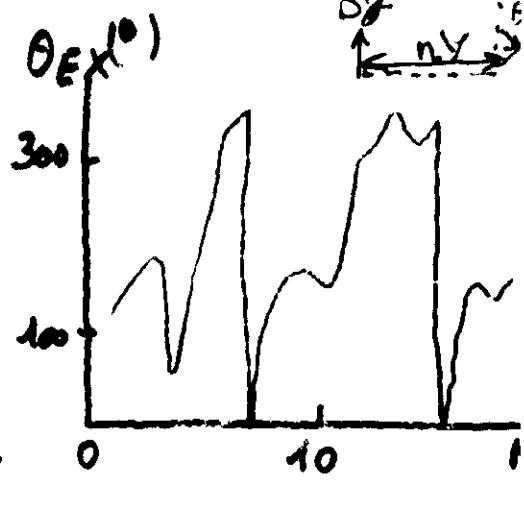


FIG. 5. Schematic representation of the basal-plane component directions in three RE superlattice systems at representative values of  $H$  and  $T$  as described in the text: (a) Gd-Y canted antiphase domain structure; (b) Dy-Y coherent, incommensurate spiral; and (c) Gd-Dy "asymmetric" state. The case of Ho-Y is similar to that of the Dy-Y except that the spiral wave vector may be locked into commensurate values corresponding to a spin-slip moment configuration. The effect of compositional modulation on the average magnitude of the moment in a given basal plane is not represented nor are possible  $c$ -axis or disorder components.

$$T_c(\text{Gd}) = 285 \text{ K}$$

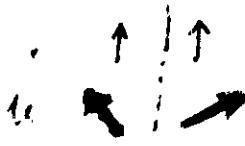
$$(Gd_{N_{Gd}} Y_{N_y})_M$$

$$T_N(\text{Dy}) = 180 \text{ K} \quad T_c(\text{Dy}) = 90 \text{ K}$$

$$N_y = 6, 10, 20$$

$$N_{Gd} = 10$$

$$1 = 200$$



cf BRUNO'S LECTURE  
FOR A DISCUSSION OF THE RESULTS  
VS EXP FOR NOSE METAL SPACERS

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### 3.6 BAND STRUCTURE CALCULATIONS

- FROM A GIVEN CRYSTALLINE STRUCTURE  
(bcc, bct, hcp, fcc...)
- USING A GIVEN EXPRESSION FOR THE EXCHANGE CORRELATION POTENTIAL
- USING ALSO SOME SIMPLIFICATIONS FOR THE POTENTIAL SHAPE TO TREAT LARGER CELLS
- CALCULATE THE ENERGY DIFFERENCE

$$\Delta E = E_F - E_{AF} = 2J(\zeta)$$

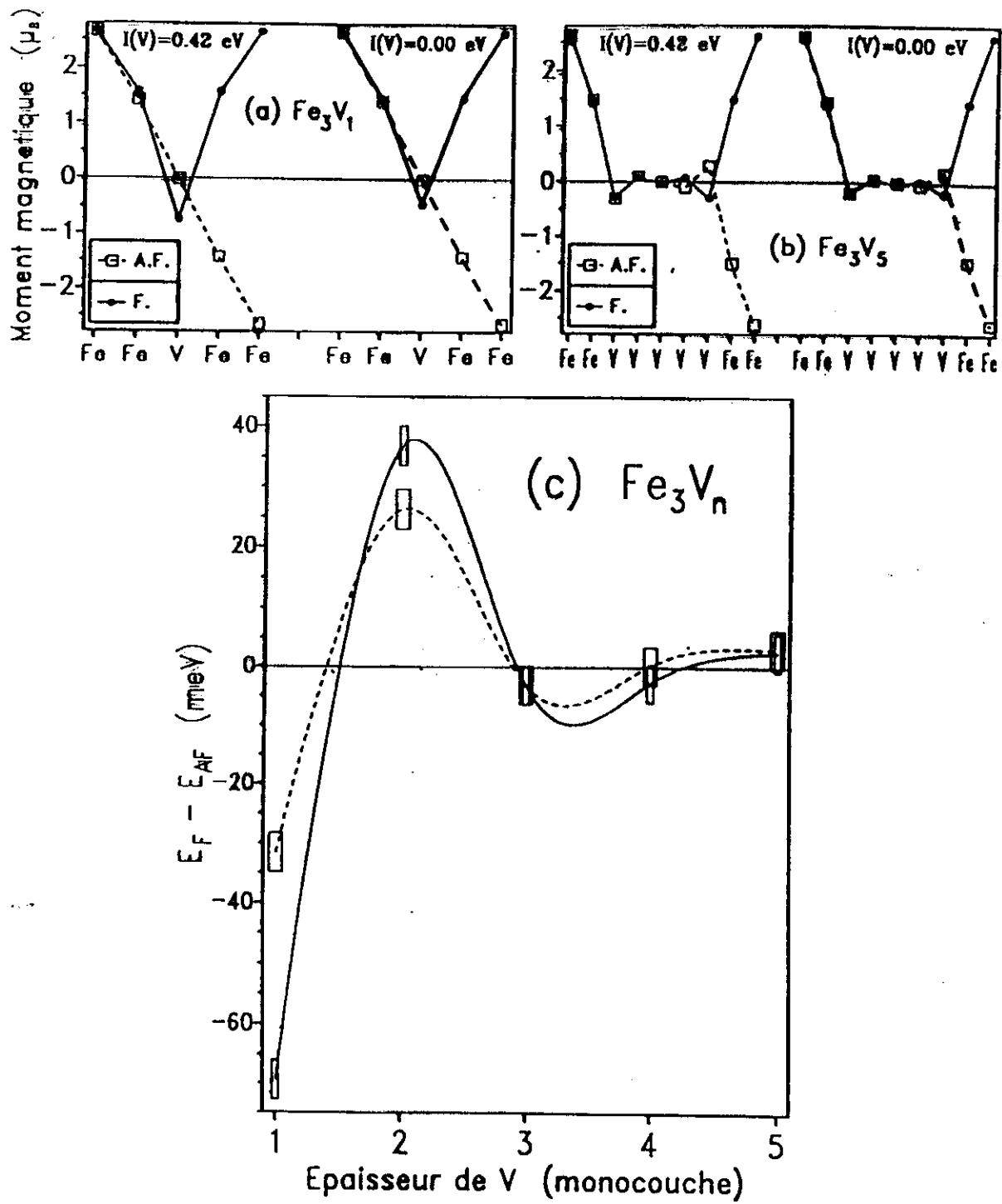
BETWEEN FERRO AND ANTIFERROMAGNET ARRANGEMENTS

→ DETERMINE THE SELF CONSISTENT BAND STRU.  
via THE LOCAL DENSITIES OF STATES

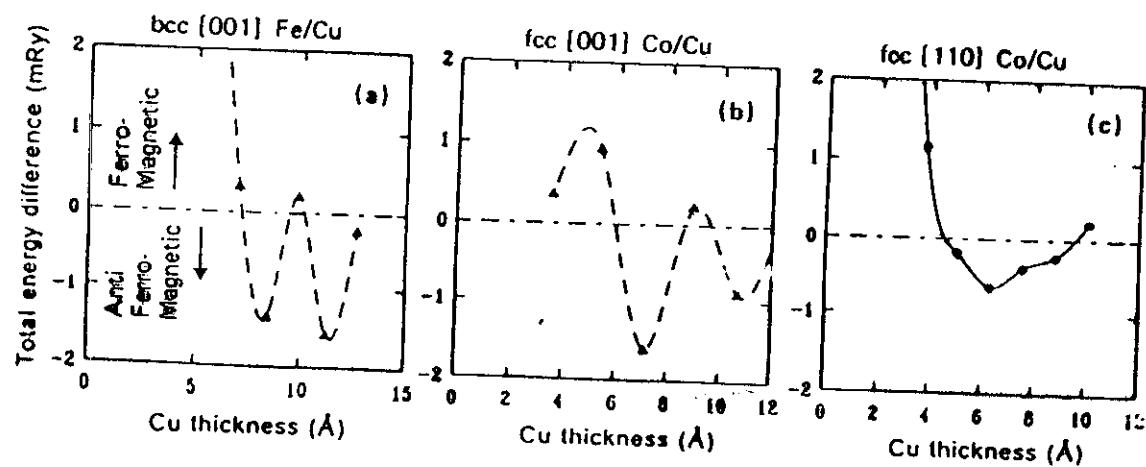
- IN THE DIRECT SPACE "TB"
- IN THE RECIPROCAL SPACE NB k POINTS

$$J(\zeta) \approx \text{meV / int. at}$$

T. E. A.



LSDA



Herman J. Strick

depends strongly on the orientation

12

## 4 A FIRST EXAMPLE : THE Pd Fe SL.

### a) EXPERIMENTAL

- Fe / Pd<sub>n</sub> (100) / Fe(100) SANDWICHES  
Celiński et al n 512  
ferromagnetic + oscillations
- Fe<sub>m</sub> Pd<sub>n</sub> SL A. Schulz et al  
ferromagn n 525
- EPITAXY BUT PRECISE STRUCTURE UNKNOWN  
starting from bcc Fe  
between Pd { fcc  
                  { fcc       $\frac{\Delta E}{E} = 0$  CAV  
   $\frac{\Delta E}{E} \sim 13\%$  BAV

### b) THEORY

- ASW CALCULATIONS
- TWO EXTREME STRUCTURES LAV CAV
- IMC — LDOS.
- DETERMINATION OF TETRAEDRALITY %

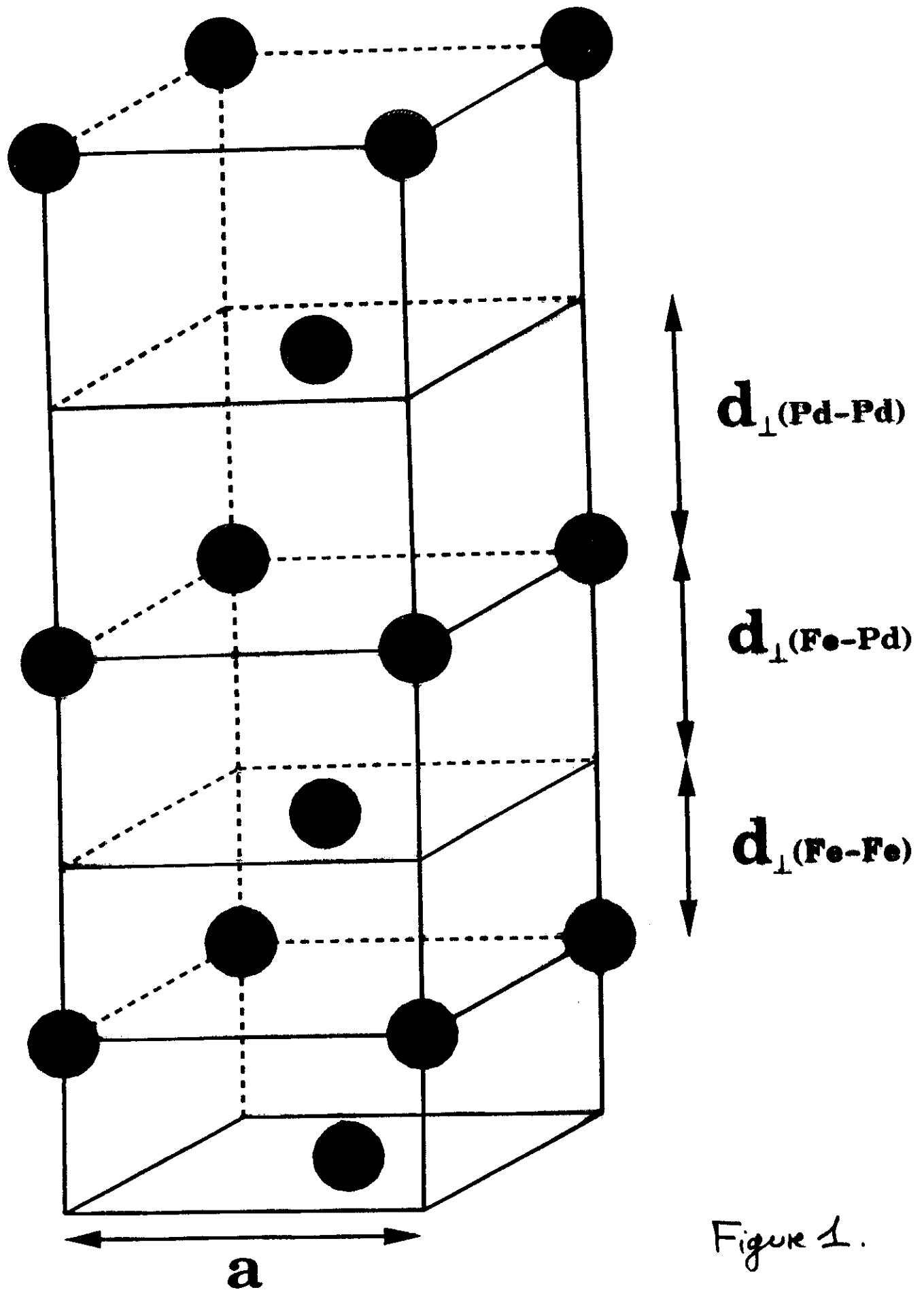


Figure 1.

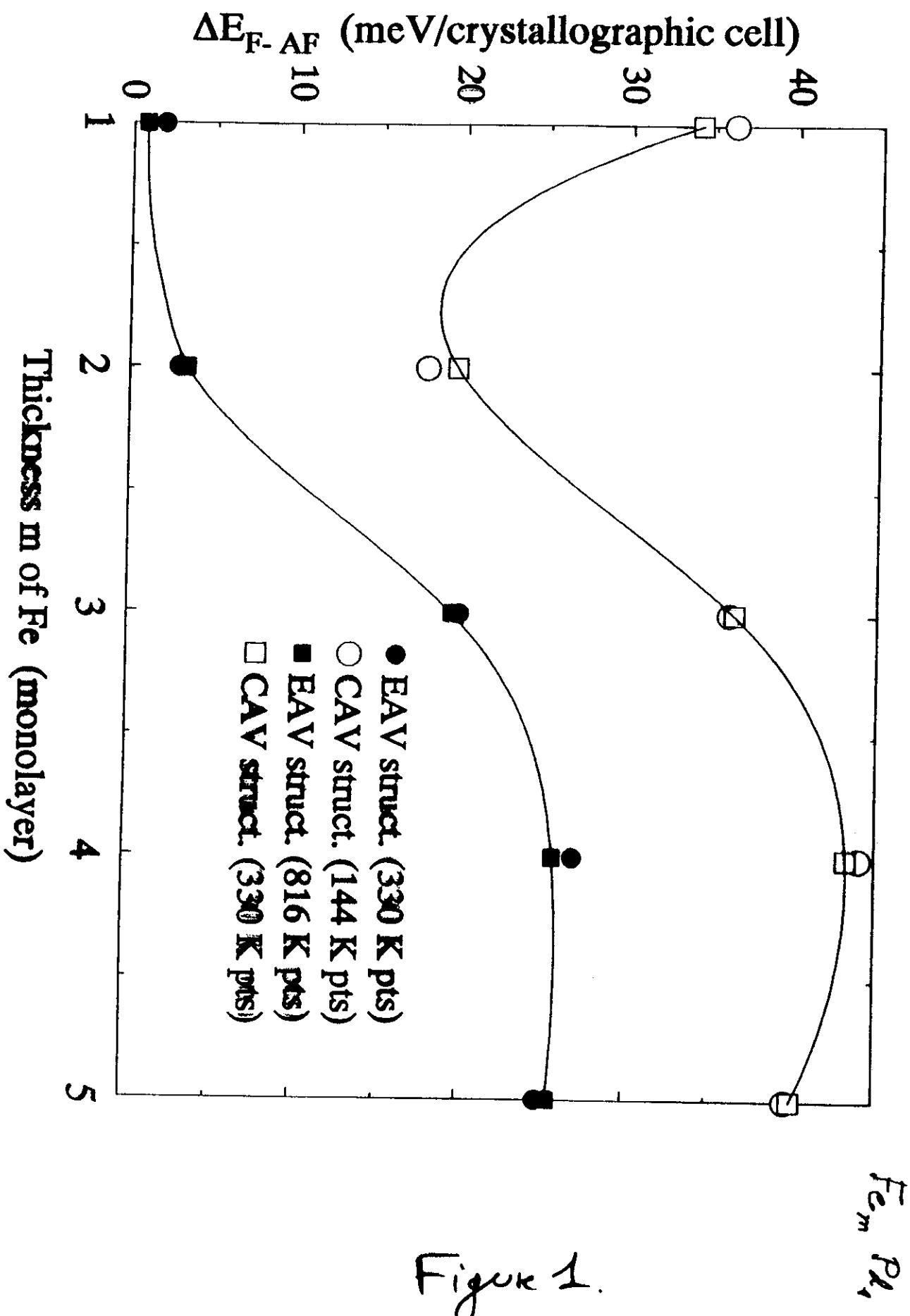


Figure 1.

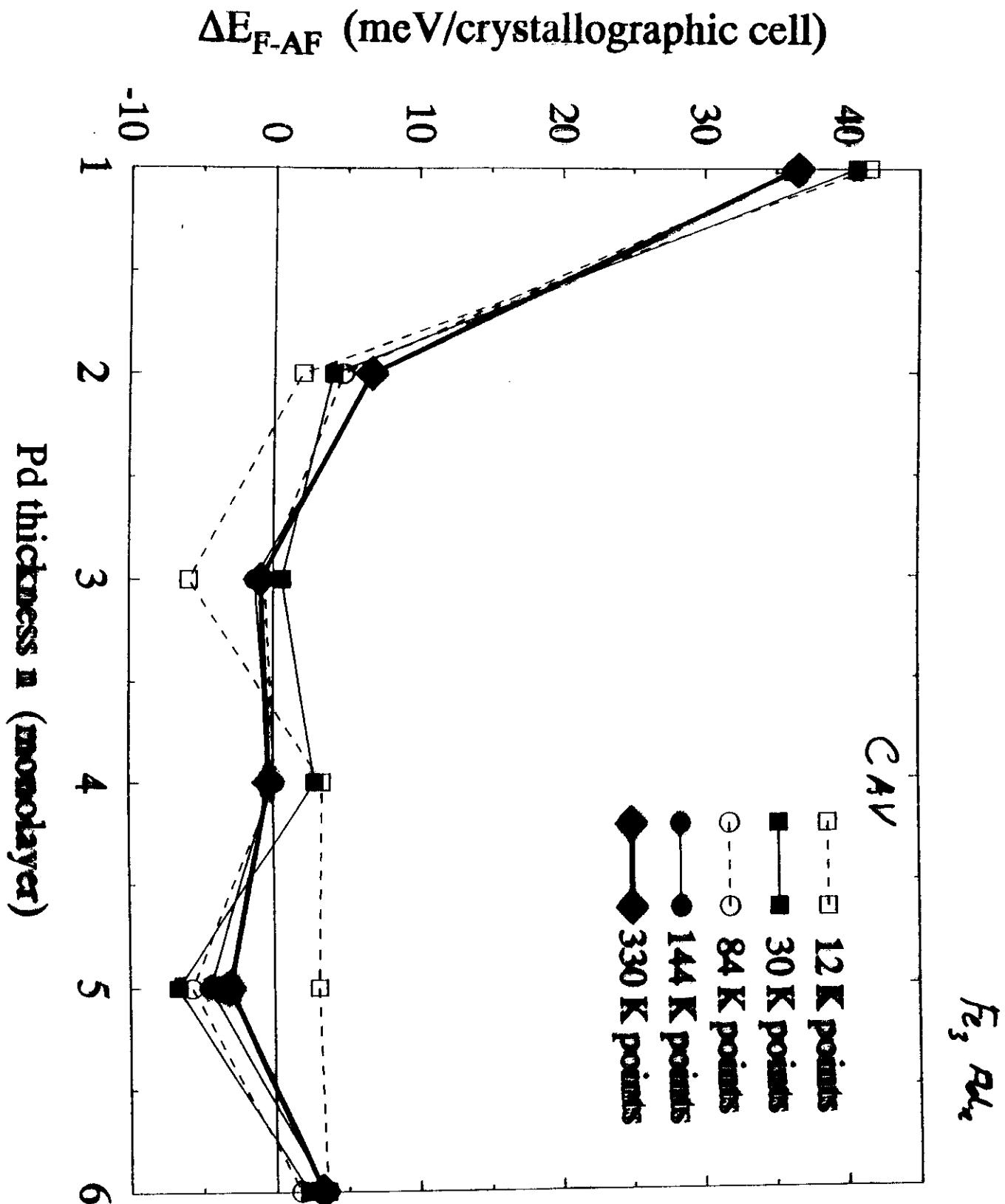


Figure 3-a

$\Delta E_{F-AF}$  (meV/crystallographic cell)

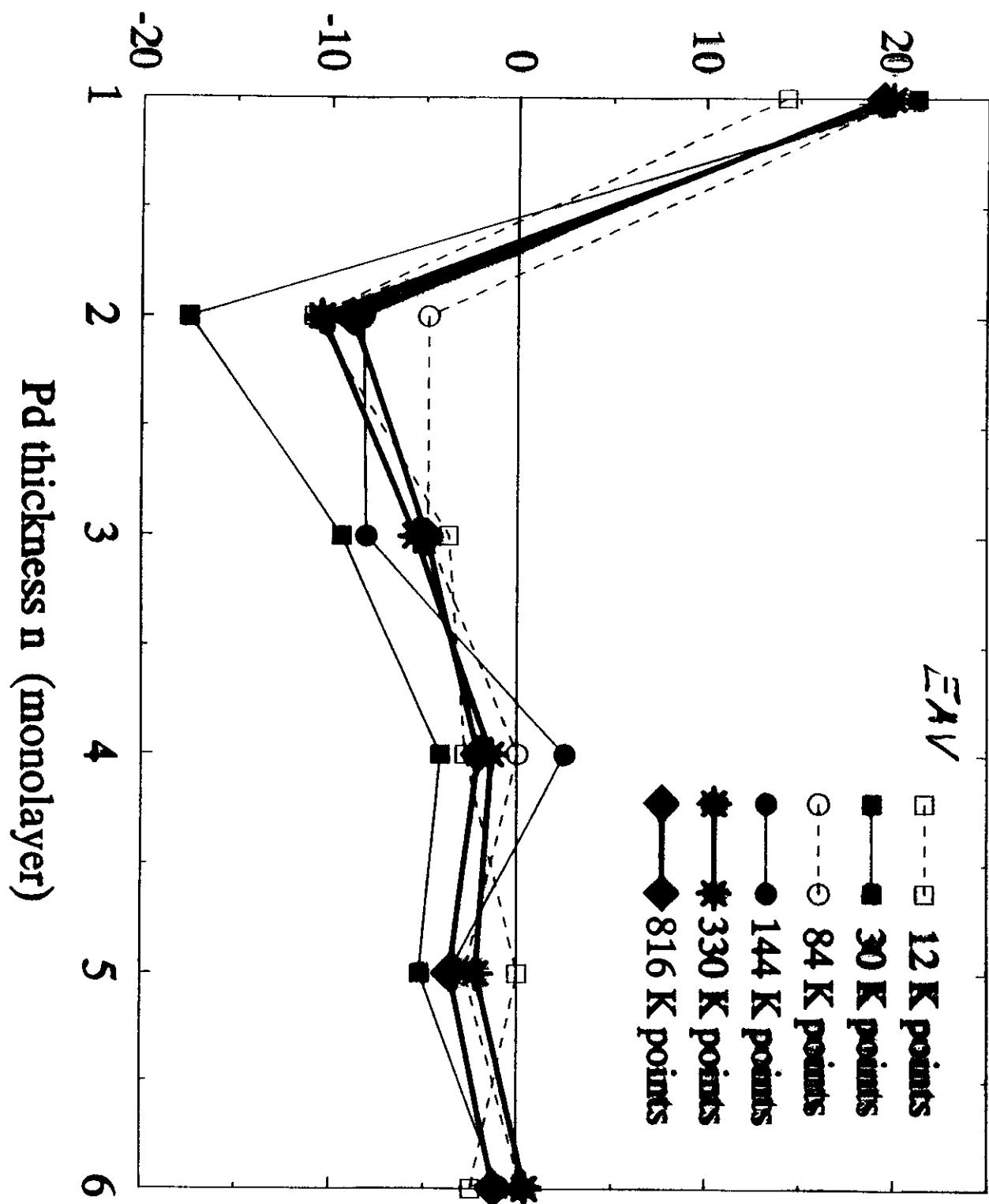


Figure 3-b

$\Delta E_{F-AF}$  (meV/crystallographic cell)

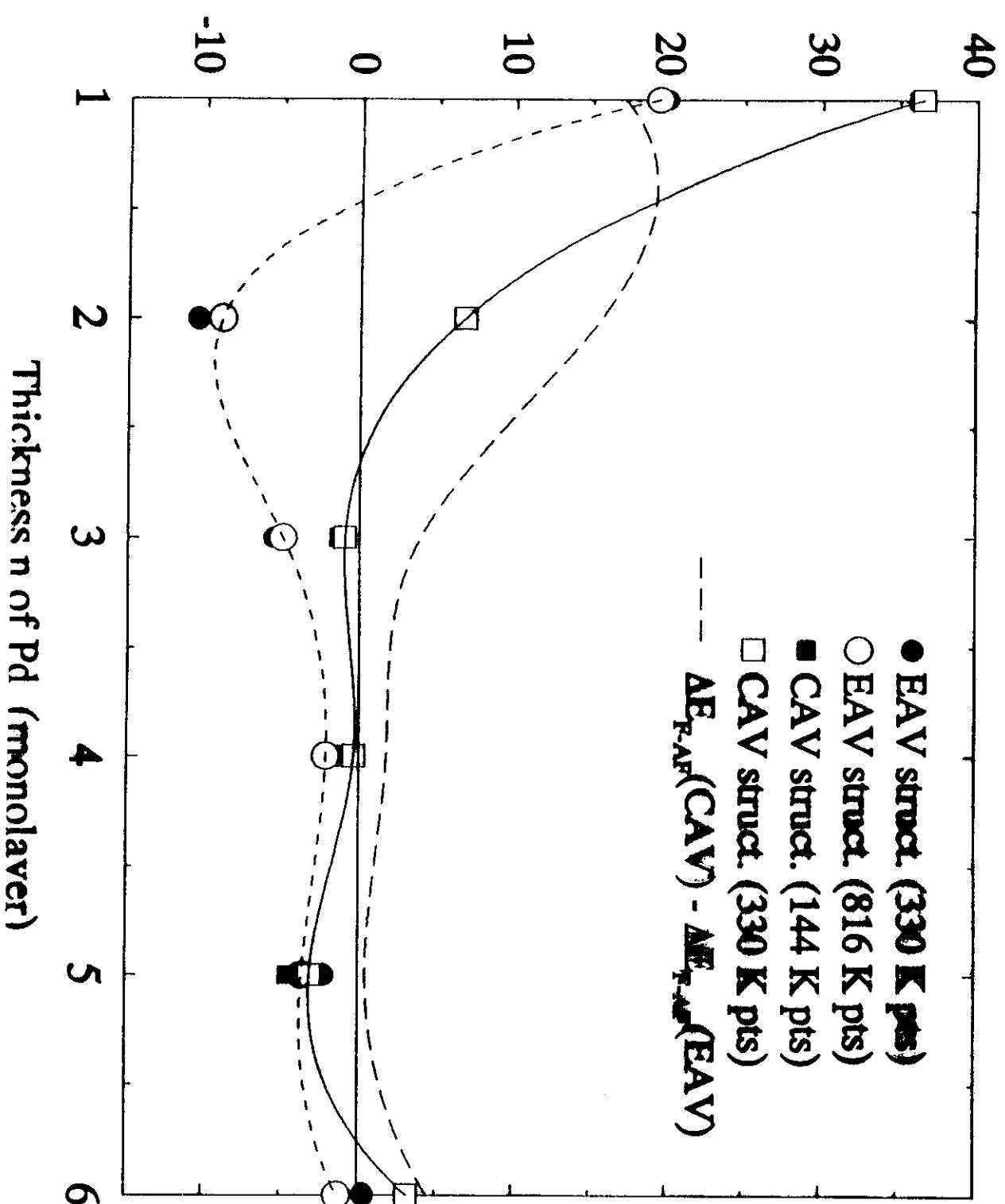


Figure 4

Figure 7  $Fe_3Pd_1$  LCO

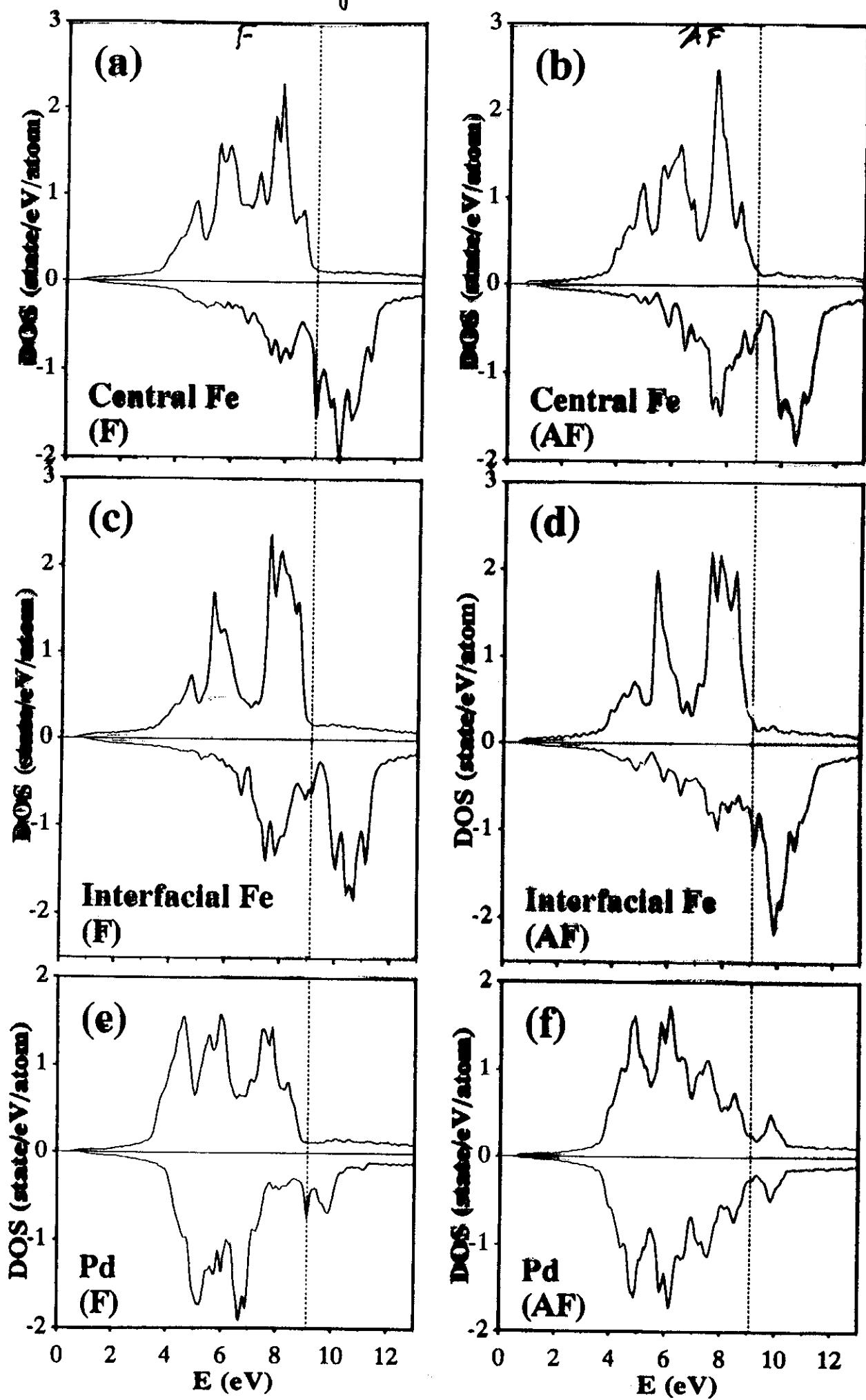


Figure 6

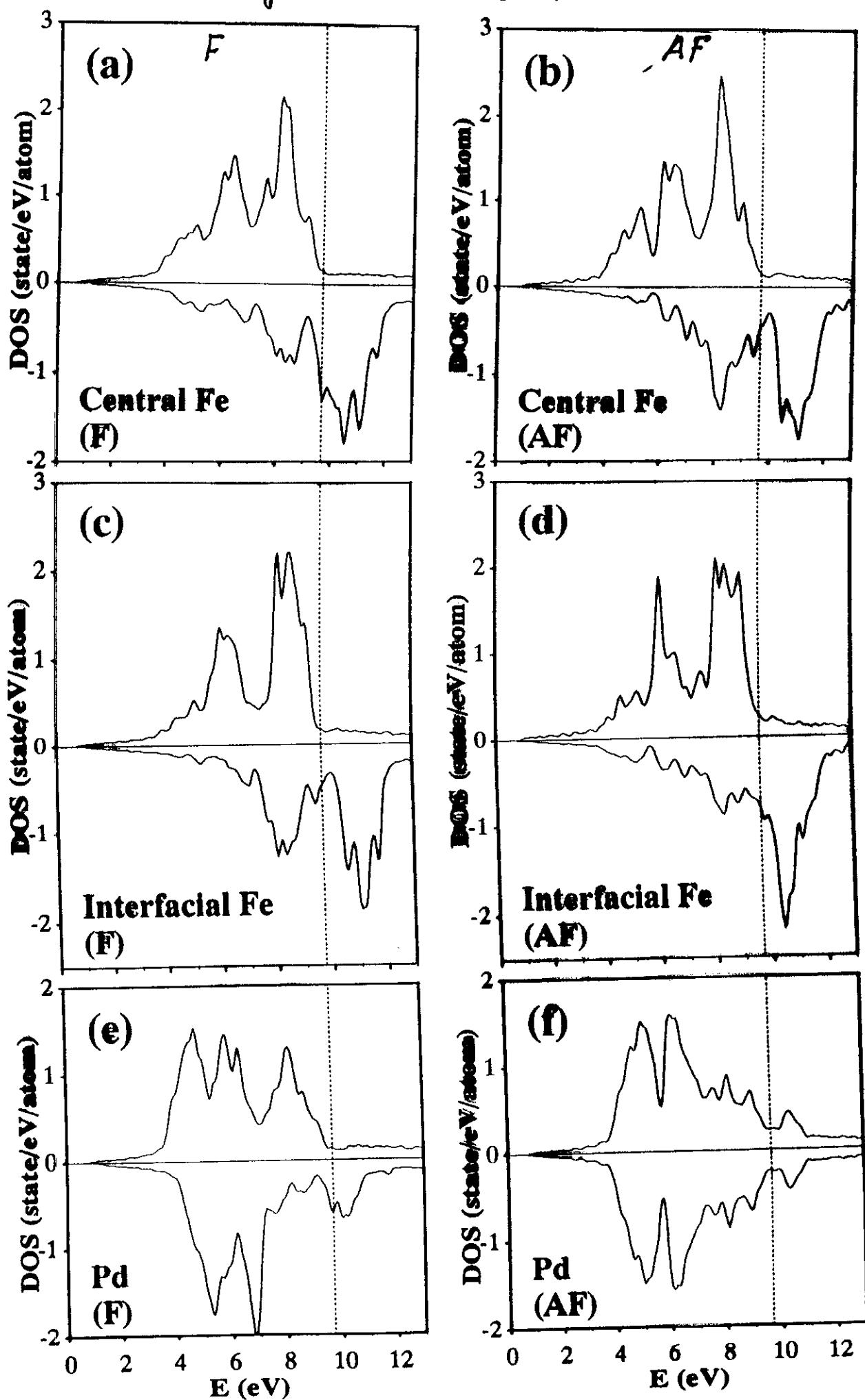
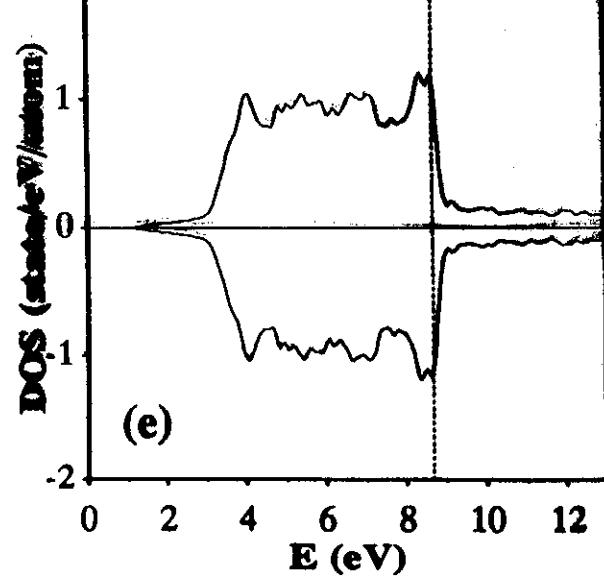
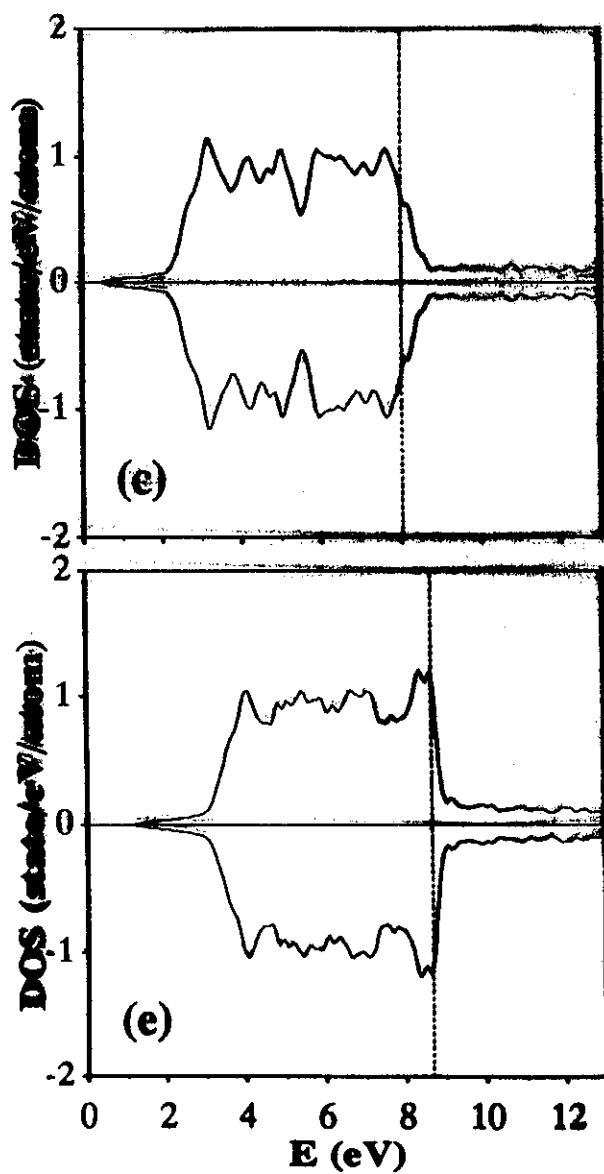
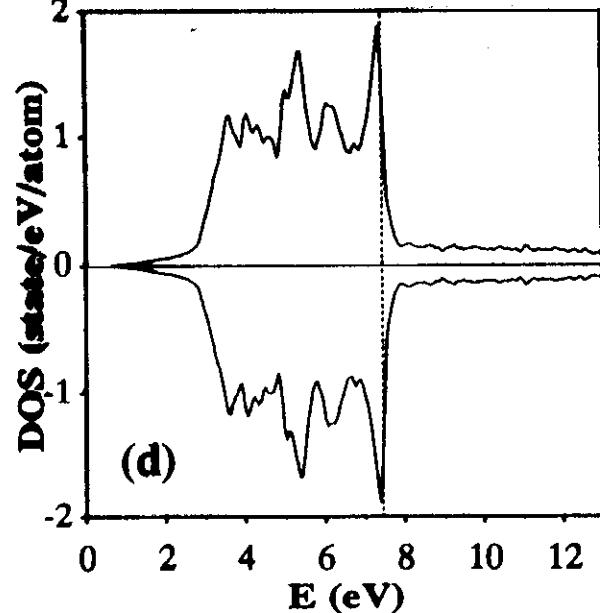
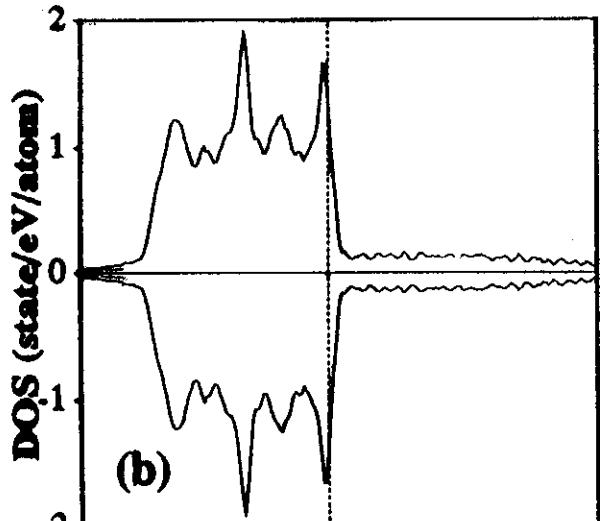
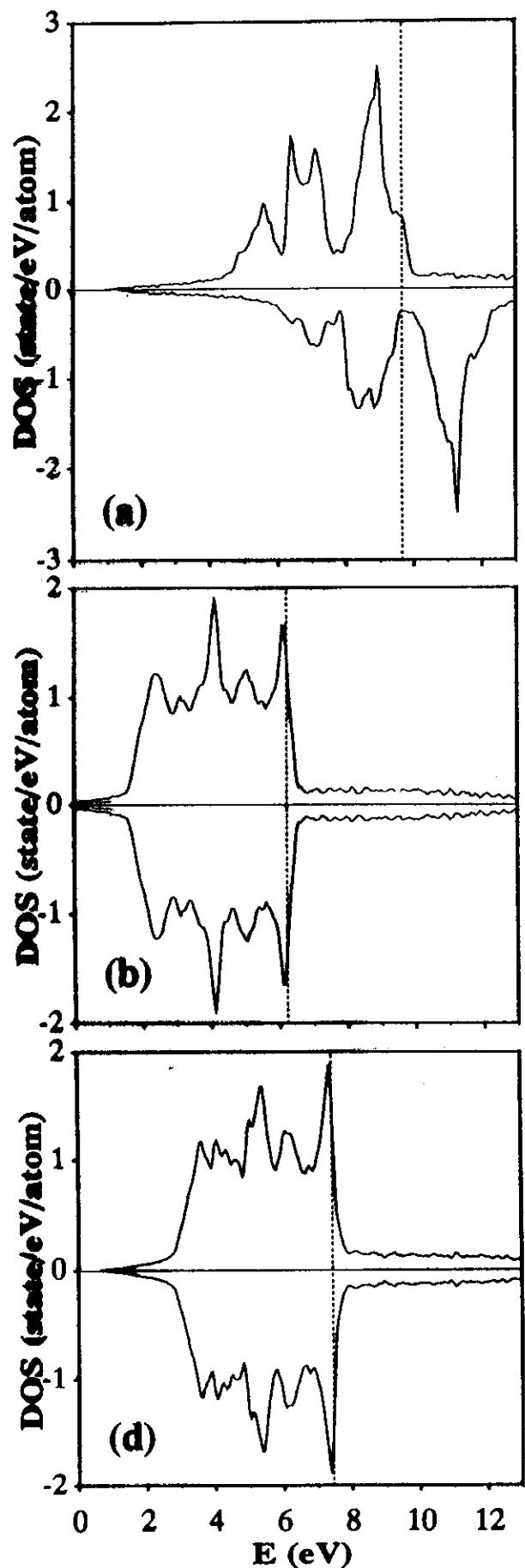
 $Fe_3Pd_4$  LCAO

Figure 8



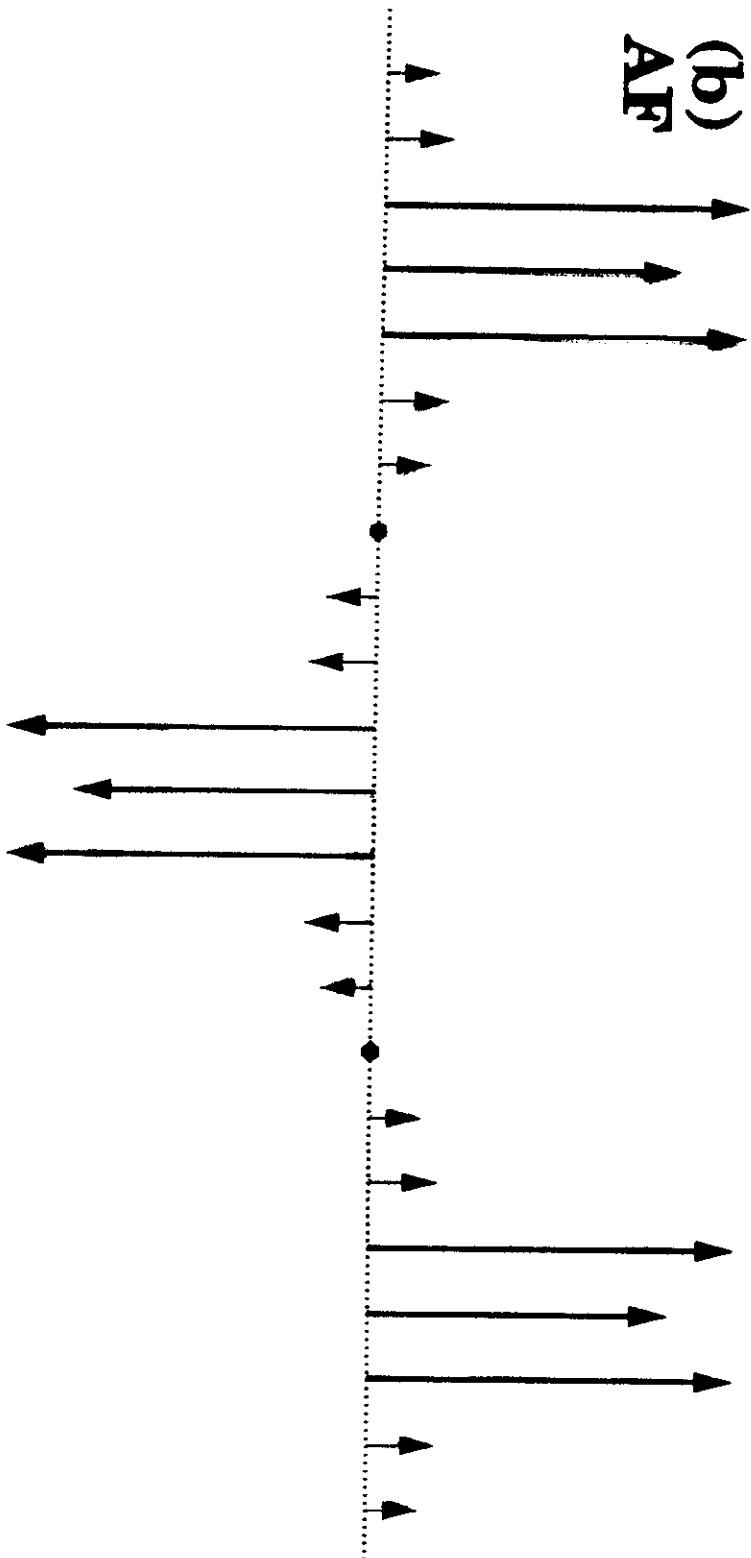
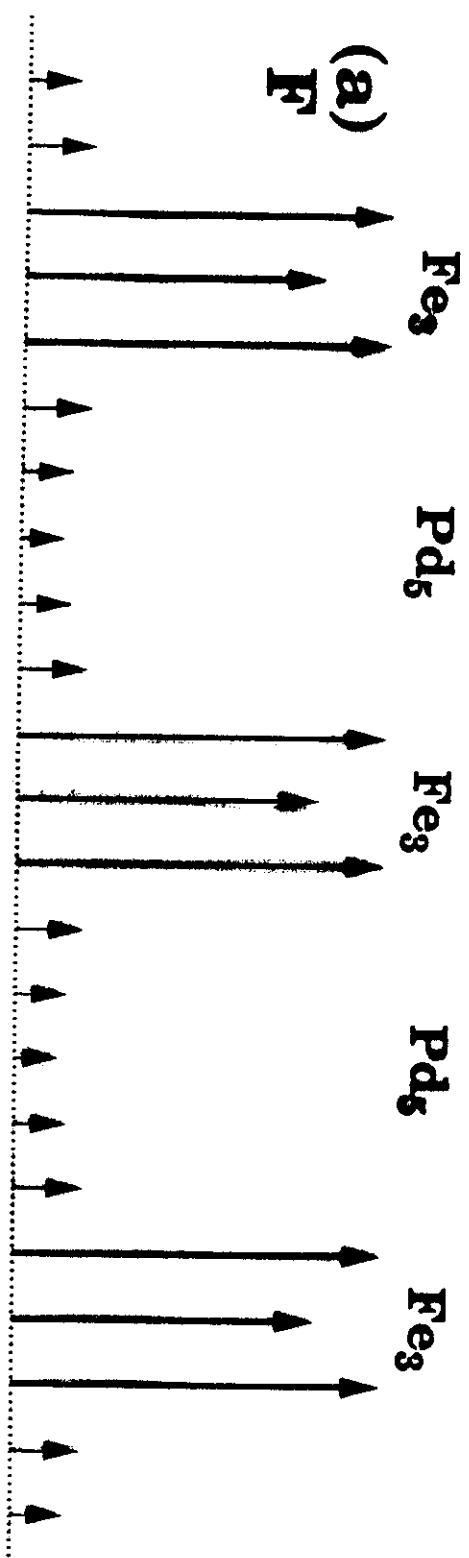
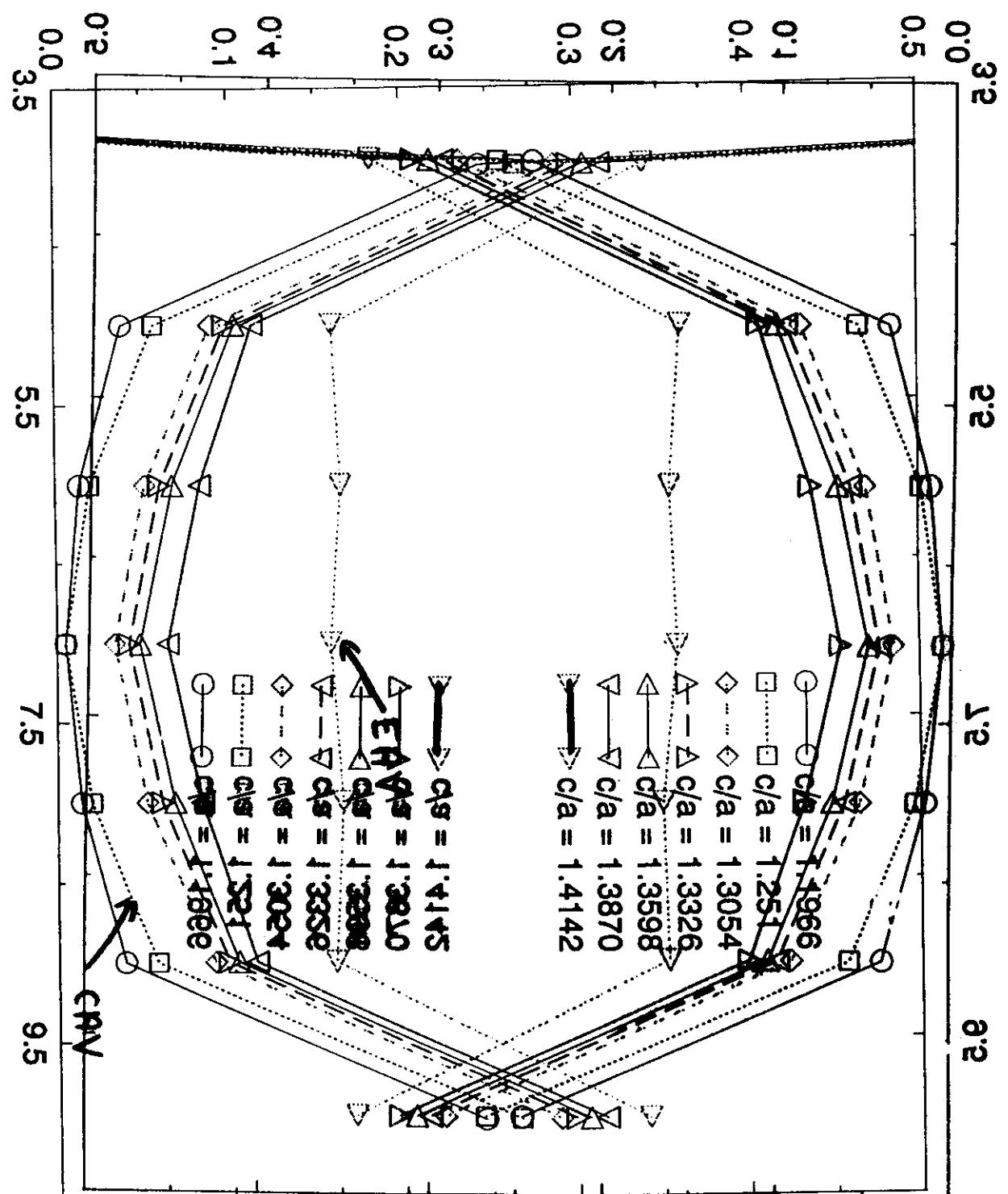


Figure 2

WT

$\text{Fe}_3\text{Pd}_2$

24



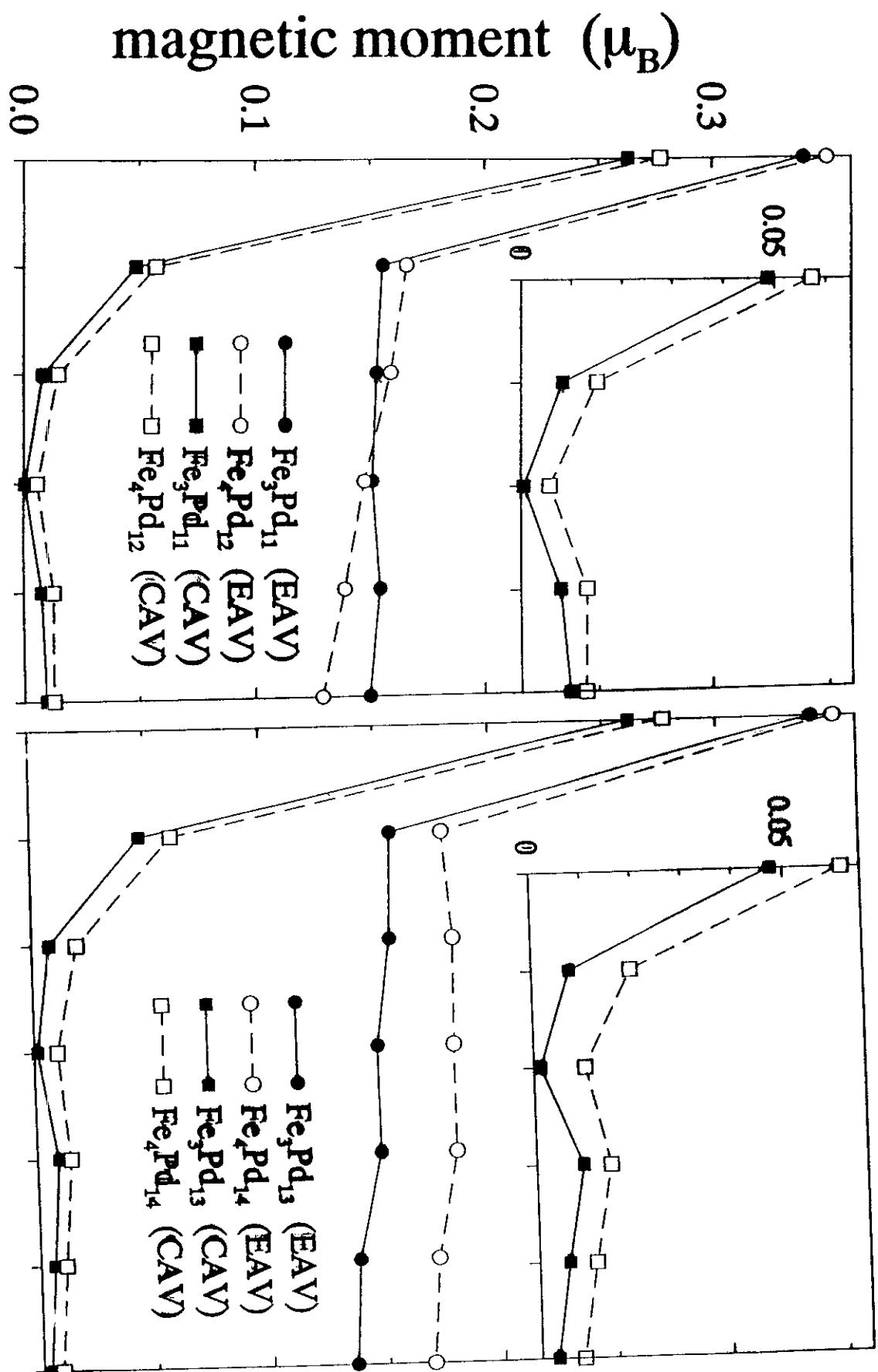
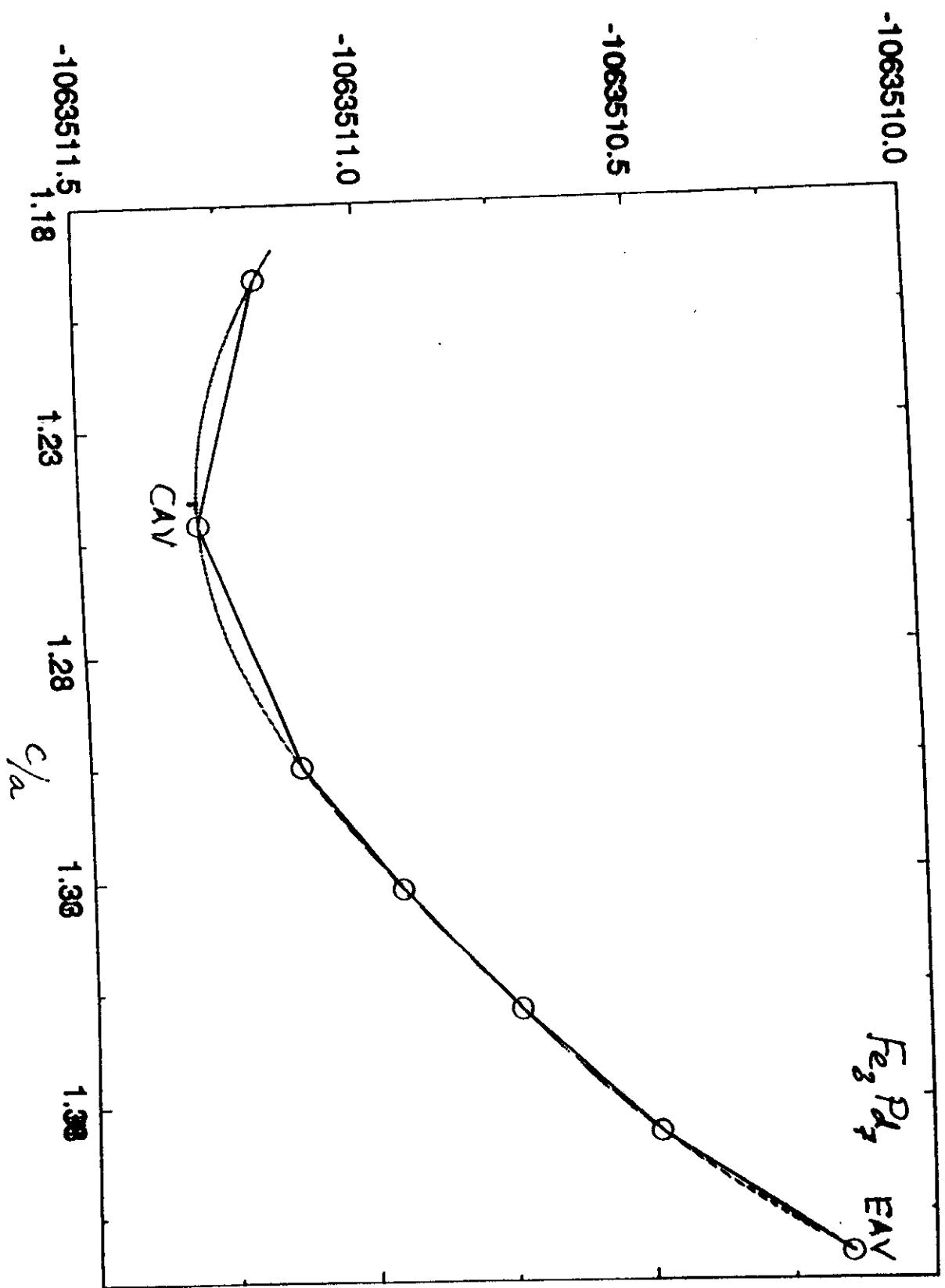
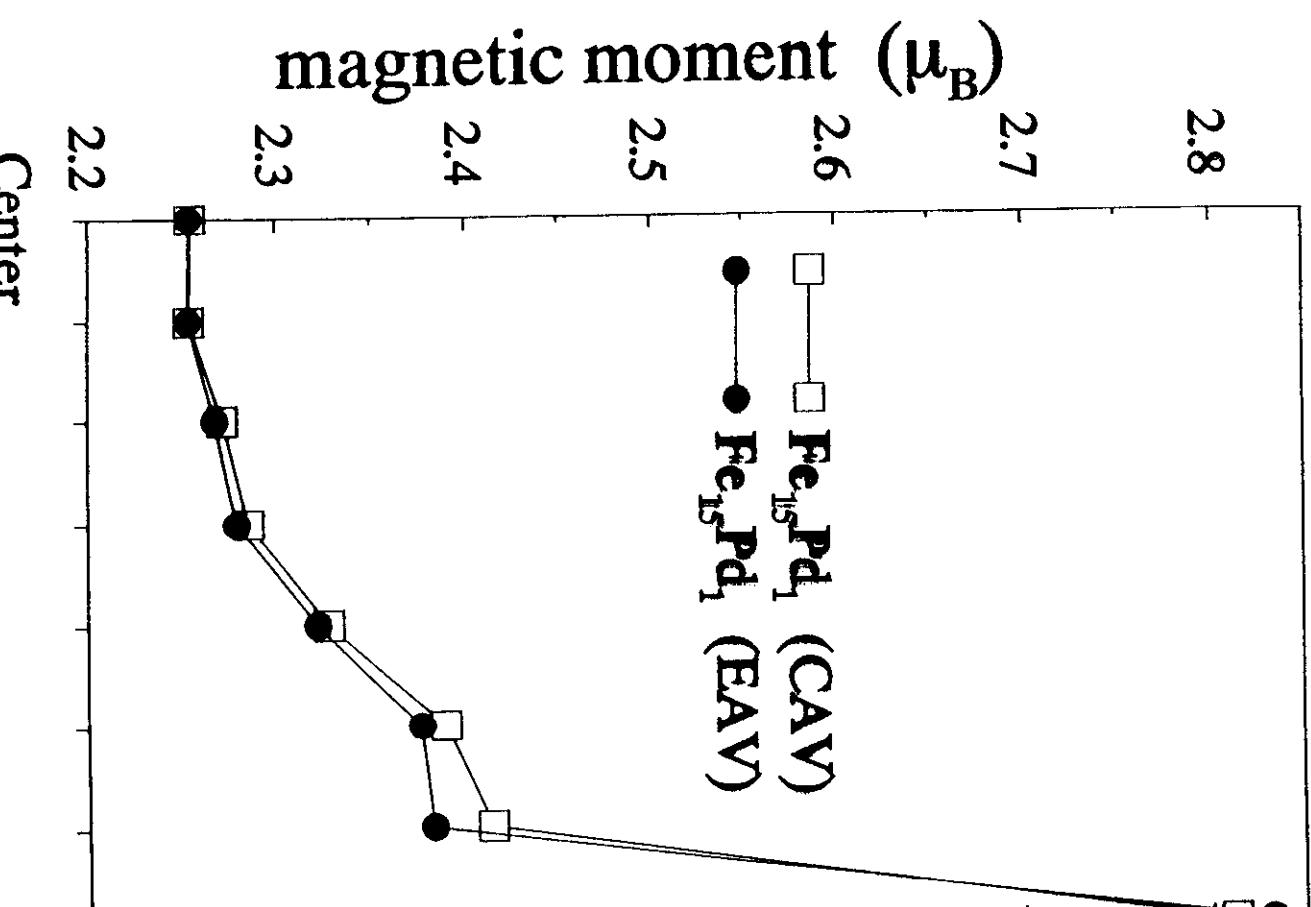


Figure 9



322 kHz

(a) Fe layer



(b) Pd layer

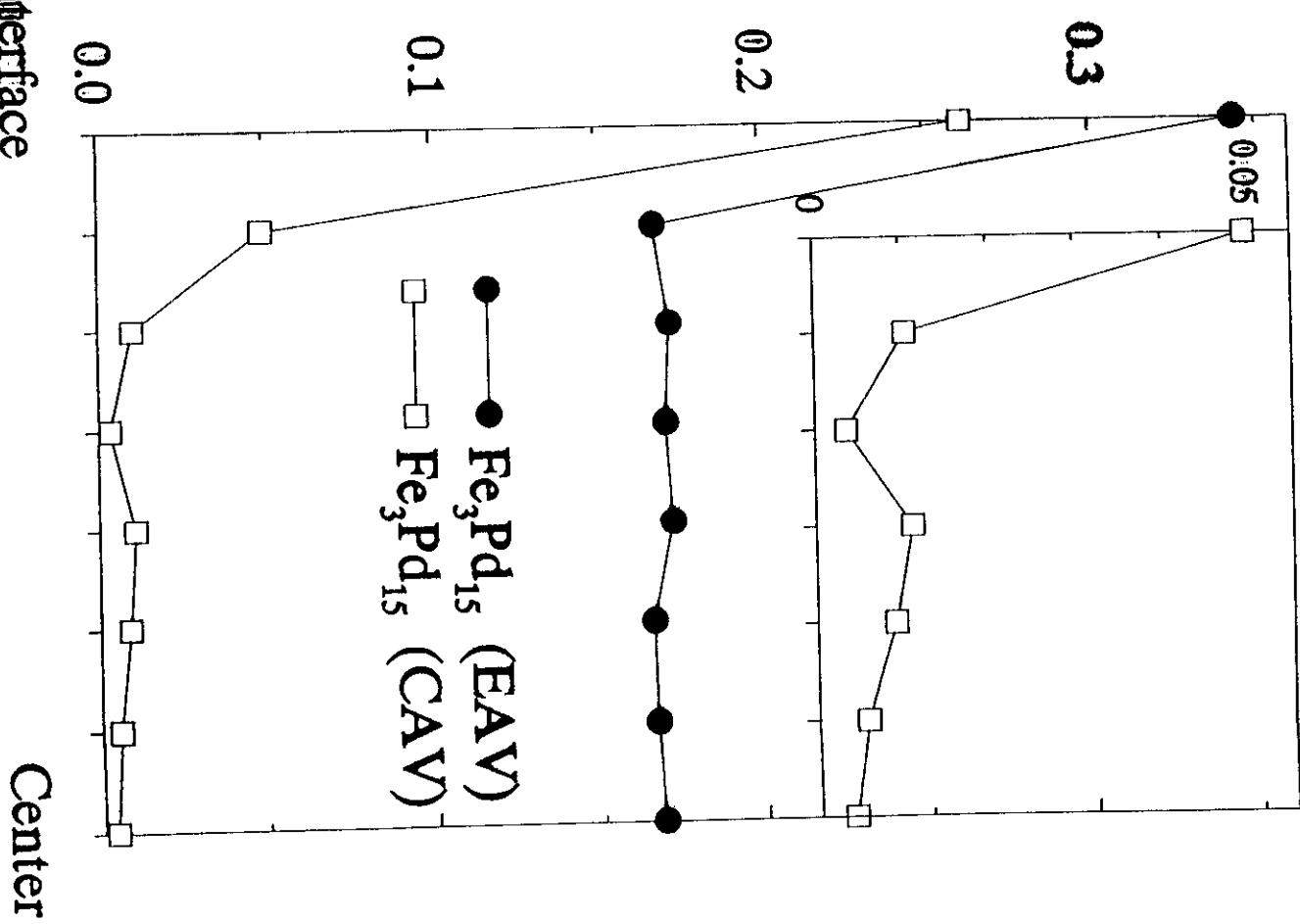


Figure 3

