ON BONDING, STABILITY AND SURFACE STATES IN ORDERED ALLOYS: FeTi AND FeAl

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Partial wave analysis together with the qualitative analysis of hybridization has been performed for two ordered alloys with CsCl structure, FeTi and FeAl. Relation to the theory of crystal superstructures and surface states is mentioned. Relative importance of covalency and ionicity in the cohesion of these compounds is treated in simple terms with the aim to better understand the nature of their stability.

The purpose of the present paper is to use the so-called qualitative theory[1,2] for the analysis of the character of bonding in two technologically interesting[3,4] ordered substitutional alloys with CsCl (B2) structure, namely FeTi and FeAl. Besides the overwhelming metallic bonding, covalency and ionicity also seem to be important here. We shall concentrate mainly on the question of the relation between the origin of the ordering phenomenon in these two alloys and the nature of bonding which can be responsible for it.

Our point of view is that covalency and ionicity survive in these alloys as a residual or fringe effect[5-7] and start to operate in the formation of the ordered phase. Both the above contributions to the cohesive energy cause the appearance of a dip in the density of states near the Fermi energy E_F during the ordered phase formation, which results in the stabilization of this phase.

The present analysis of both investigated alloys is based on the non-selfconsistent APW band-structure calculations[8] where the $3d^n\,4s^1$ configurations of transition metal atoms ($n = 3$ for Ti, $n = 7$ for Fe) and full Slater exchange were employed in the construction of the crystal potential. Such calculations are, as a rule, in good agreement with the selfconsistent calculations using a better treatment of exchange[9-11], especially in case of transition metal aluminides[12-14], and it seems, therefore, that the effect of self-consistency might be as well simulated in this way. Indeed, the band structures[8] are very close to the fully selfconsistent ones of FeTi (ref.[11]) and FeAl (ref.[12]) and the differences turned out not to be important for the present purpose.

THEORETICAL

From the methodological point of view, the analysis of the band structure of FeTi differs from that of FeAl. The former alloy is composed of two different transition metals and the ordering can be formally considered as a superstructure effect[1,15–18] imposed on a BCC transition metal band structure. The latter is obtained by ignoring the difference between Fe and Ti in the alloy. If this difference is switched on, the BCC symmetry is reduced to the CsCl one and Bloch states with wave vectors differing by a reciprocal lattice vector of the new lattice start to interact. High symmetry directions of the Brillouin zone (BZ) are especially instructive for the illustration of this effect, since it can be (in most simple cases) reduced to the simple folding of the energy branches of the old BCC Brillouin zone around planes perpendicular to any $\Delta(\Gamma\text{-H})$ direction and going through its midpoint (*i.e.* reflecting H into Γ). These planes form the boundary of the BZ of the new CsCl lattice. When the folded branches cross, a gap opens between them due to the non-crossing rule, if the interaction is not symmetry forbidden. As a good example explaining the above effects, one can take the band structure of BCC Cr[16–18], which during the antiferromagnetic phase transition goes over into a superstructure band structure closely resembling that of FeTi. Results of the present paper which are based on the partial analysis of the wave function of FeTi, enabled a deeper understanding of the origin of ordering in this alloy. Naturally, as far as ordering is concerned, ordered alloys are formally equivalent to antiferromagnets in the Ising model.

With FeAl, the analysis is slightly more complicated since one of the two atoms is a normal metal atom and there are no reasons to base the analysis on the BCC transition metal band structure as a starting point. Hence, it is necessary to carry out the surface projections[1,2,7] directly from the band structure of the alloy in order to find the gaps which can be responsible for the ordered phase formation. A detailed analysis of this kind has been performed[7] elsewhere for β'-CuZn. Here, we illustrate the results on a different system from the β'-brass family.

We shall distinguish between two types of gaps, hybridizational (HG) and non-hybridizational (NHG). By definition, a HG corresponds to a situation when by moving along a certain direction in BZ, the character of the wave function changes for both energy branches which delimite this HG, the lower one and the upper one. Numerous illustrations of this situation can be found in the Tables below. As to the formal definition of the HG based on the crossing of two originally non-interacting $E^0(\boldsymbol{k})$ branches (corresponding to non-interacting Bloch states based on a certain type of localized orbitals, *e.g.* *s*, *p* or *d* located on atoms A or B in the AB alloy), see elsewhere[1,2,7]. Gaps which are not HG, are NHG by definition.

In the present paper, a HG is related to the concept of chemical bonding (covalency) since the underlying hybridization creates bonding and antibonding energy branches[19,20]. The strength of the covalency depends upon *a*) the extension of the respective

HG in $\boldsymbol{k}$-space; *b*) the occupancy of the bonding (lower) and antibonding (upper) branches belonging to it, *i.e.* upon the relative position of E_F with respect to this HG.

The ionicity often arises from a favourable position of E_F in a HG, the lower edge

TABLE I

Partial wave analysis for two energy branches delimiting the NHG in Δ_2 states of FeTi. Irreducible representations (IR), energy (E) from ref.[8] and partial charges (C) inside the muffin-tin spheres (Ti or Fe). The "missing" charge (to 100%) falls essentially outside the muffin-tin spheres. $E_F = 0.69$ Ry for FeTi

Point:	Γ	Δ (middle)	X
IR	12	2	3′
E(Ry)[a]	0·8271	0·8055	0·7358
C(Ti)%	59·105e_g	61·786e_g	77·073e_g
C(Fe)%	31·986e_g	23·134e_g	0
IR	12	2	2
E(Ry)	0·4423	0·4829	0·5395
C(Ti)%	19·152e_g	15·533e_g	0
C(Fe)%	61·404e_g	66·393e_g	86·026e_g

[a] 1 Ry = 2·178 . 10^{-18} J.

TABLE II

Partial wave analysis for two energy branches delimiting the NHG in Δ_2 states of FeTi

Point:	Γ	Δ (middle)	X
IR	25′	2′	2′
E(Ry)	1·0086	1·0002	0·9731
C(Ti)%	86·632t_{2g}	89·204t_{2g}	94·408t_{2g}
C(Fe)%	10·292t_{2g}	6·360t_{2g}	0
IR	25′	2′	3
E(Ry)	0·6166	0·6321	0·6456
C(Ti)%	8·469t_{2g}	5·382t_{2g}	0
C(Fe)%	88·337t_{2g}	91·307t_{2g}	96·667t_{2g}

of which derives mostly from more electronegative atoms, while the upper edge comes from more electropositive atoms.

TABLE III

Partial wave analysis for two energy branches delimiting the NHG in Δ_5 states of FeTi

Point:	Γ	Δ (middle)	X
IR	25′	5	5′
E(Ry)	1·0086	0·9335	0·8522
C(Ti)%	86·632t_{2g}	76·388t_{2g} 1·107p	80·568t_{2g}
C(Fe)%	10·292t_{2g}	5·936t_{2g} 5·363p	6·663p
IR	25′	5	5
E(Ry)	0·6166	0·6173	0·6107
C(Ti)%	8·469t_{2g}	6·485t_{2g} 0·820p	1·936p
C(Fe)%	88·337t_{2g}	88·031t_{2g} 0·022p	92·205t_{2g}

TABLE IV

Partial wave analysis for two energy branches delimiting the NHG in Σ_3 states of FeTi

Point:	Γ	Σ (middle)	M
IR	25′	3	5
E(Ry)	1·0086	0·9153	0·9890
C(Ti)%	86·632t_{2g}	83·623t_{2g} 0·227p	73·749t_{2g}
C(Fe)%	10·292t_{2g}	2·111t_{2g} 4·210p	22·648t_{2g}
IR	25′	3	5
E(Ry)	0·6166	0·6297	0·5481
C(Ti)%	8·469t_{2g}	0·927t_{2g} 1·097p	16·552t_{2g}
C(Fe)%	88·337t_{2g}	92·430t_{2g} 0·161p	76·627t_{2g}

RESULTS AND DISCUSSION

FeTi Alloy

First, let us sketch shortly the way in which HG and NHG are found in the band structure of this type of alloy. As mentioned above, the folding of BCC energy bands enables to predict the opening of new gaps caused by the lowering of symmetry during the ordering transition to the CsCl structure. It also indicates which type of branches of the original BCC band structure is responsible for this effect. At first sight, it might seem possible to apply the formal HG definition to each such crossing and to say

TABLE V

Partial wave analysis for three energy branches delimiting two HG in Λ_1 states of FeTi

Point:	Γ	Λ (middle)	R
IR	25′	1	1
E(Ry)	1·0086	0·9316	1·3190
C(Ti)%	86·632t_{2g}	59·357t_{2g} 4·316s 1·282p	0
C(Fe)%	10·292t_{2g}	17·978t_{2g} 0·445s 5·059p	74·538s
IR	25′	1	15
E(Ry)	0·6166	0·5738	0·6108
C(Ti)%	8·469t_{2g}	11·808t_{2g} 1·038s 0·624p	55·459t_{2g}
C(Fe)%	88·337t_{2g}	72·770t_{2g} 3·639p 0·002s	19·411p
IR	1	1	25′
E(Ry)	0·1808	0·4076	0·5289
C(Ti)%	26·313s	3·974t_{2g} 14·629s 8·082p	7·299p
C(Fe)%	34·152s	5·025t_{2g} 23·548s 7·749p	82·436t_{2g}

that it must lead to a HG. However, this is not the case, because the above branches do not fulfill the basic assumption of being non-interacting with respect to the interaction of A and B sublattice. Namely, in the BCC lattice, the branches are already mixed (hybridized). Hence, the crossing need not lead to a HG but can lead to a NHG, one edge of which being formed mainly by A derived states and the other by B derived states. It appears therefore, that it is necessary to have at one's disposal the partial wave analysis of the wave functions of the investigated alloy and to use it simultaneously with the definition of the HG given in the Theoretical. Hence, for

TABLE VI

Partial wave analysis for four energy branches delimiting three HG in Λ_3 states of FeTi

Point:	Γ	Λ (middle)	R
IR	25′	3	12′
E(Ry)	1·0086	0·9415	1·0315
C(Ti)%	86·632t_{2g}	70·294d[a] 0·004p	97·926t_{2g}
C(Fe)%	10·292t_{2g}	16·587d 2·556p	0
IR	12	3	12
E(Ry)	0·8271	0·8282	0·6695
C(Ti)%	59·105e_g	48·201d 3·123p	0
C(Fe)%	31·986e_g	30·502d 6·026p	98·673e_g
IR	25′	3	15
E(Ry)	0·6166	0·5732	0·6108
C(Ti)%	8·469t_{2g}	13·330d 1·225p	55·459t_{2g}
C(Fe)%	88·337t_{2g}	76·876d 0·390p	19·411p
IR	12	3	25′
E(Ry)	0·4423	0·5402	0·5289
C(Ti)%	19·152e_g	10·086d 3·082p	7·299p
C(Fe)%	61·404e_g	64·481d 4·171p	82·436t_{2g}

[a] $d = e_g + t_{2g}$.

FeTi we proceed as follows[21]: The band structure of Cr along a high symmetry direction is folded back as described above and the resulting band structure is identified with that obtained for FeTi by direct calculation. The respective partial wave analysis is then used to decide whether the newly opened gaps are HG or NHG. They are HG, if the character of both the branches delimiting the gap interchanges by moving along the high symmetry direction.

Let us illustrate the whole procedure on the most important new gaps located in the neighbourhood of E_F. First, let us consider NHG. There are four of them, in Δ_2, $\Delta_{2'}$, Δ_5 and Σ_3 states; their partial wave analysis is given in Tables I–IV. The typical behaviour is that the lower branch of any of these gaps belongs mainly to Fe, the upper to Ti atoms, both having a $d(t_{2g}$ or $e_g)$ character. Similar situation is found also with Σ_2 (mainly t_{2g} character) and Σ_4 (mainly e_g character) NHG at E_F. The opening of the Σ_3 NHG has been observed experimentally[17] with Cr during the antiferromagnetic phase transition. Our results are in general agreement with those for FeCo (ref.[15]) for the NHG along Δ, taking into account the fact that the order of electronegativities in FeCo is reversed with respect to that in FeTi.

TABLE VII

Partial wave analysis for two energy branches delimiting the HG in Δ_1 states of FeAl. $E_F =$ = 0·71 Ry for FeAl

Point:	Γ	Δ (middle)	X
IR	15	1	1
E(Ry)	1·1236	0·8677	0·8046
C(Fe)%	17·510p	52·196e_g 5·502s 4·751p	86·277e_g 6·085s
C(Al)%	53·391p	0·757e_g 18·278p 5·794s	3·068p
IR	12	1	1
E(Ry)	0·5475	0·5092	0·2691
C(Fe)%	77·001e_g	40·721e_g 5·781p 2·343s	9·680e_g 23·128s
C(Al)%	5·982e_g	5·376e_g 13·981p 4·152s	31·974p

The ionicity arises since due to the superstructure effect (folding), any original branch of the BCC band structure is split into two parts, the lower (mainly occupied) one belonging to more electronegative atoms and the upper (empty) one belonging to more electropositive atoms. This fact is confirmed by calculations of ref.[11] in which a 0·18 electron transfer of mainly d character takes place from Ti to Fe.

Next, let us discuss the HG. They lie in Λ_1 and Λ_3 states. The related partial wave analysis is found in Tables V, VI.

In Λ_1 states there are two HG, the higher one being around E_F (Table V). In the picture of non-interacting $E^0(\boldsymbol{k})$ branches, one can imagine that the lower HG results from the crossing of the wide s(Fe) $\Gamma_1 - \Lambda_1 - R_1$ branch with the t_{2g}(Fe) $\Gamma_{25'}$ (lower) $- \Lambda_1 - R_{25'}$ one. The higher HG arises from the crossing of the above mentioned s(Fe) branch with the t_{2g}(Ti) $\Gamma_{25'}$ (upper) $- \Lambda_1 - R_{15}$ branch.

As expected, the partial wave analysis of Tables V confirms the above picture and shows clearly the change of the character along the branches considered, as required for HG. Analogous situation is found for Δ_1 states (see Fig. 1 and Table VII of ref.[15]), where t_{2g} states of Λ_1 should be replaced by e_g states.

In Λ_3, three HG are present. The middle one around E_F is the largest and the most important of the three. The lower HG can be imagined as the result of the crossing of the following $E^0(\boldsymbol{k})$ branches: an e_g(Fe) type Γ_{12} (lower) $- \Lambda_3 - R_{12}$ branch with

TABLE VIII

Partial wave analysis for two energy branches delimiting the HG in Σ_4 states of FeAl

Point:	Γ	Σ (middle)	M
IR	15	4	2
E(Ry)	1·1236	0·8997	0·7672
C(Fe)%	17·510p	58·031e_g 7·577p	97·952e_g
C(Al)%	53·391p	1·364e_g 20·354p	0
IR	12	4	5′
E(Ry)	0·5475	0·5537	0·5272
C(Fe)%	77·001e_g	38·248e_g 8·733p	18·852p
C(Al)%	5·982e_g	4·215e_g 20·062p	43·231p

a t_{2g}(Fe) type $\Gamma_{25'}$ (lower) − Λ_3 − $R_{25'}$ branch. The middle HG appears due to the crossing of the above e_g(Fe) branch with the t_{2g}(Ti) $\Gamma_{25'}$ (upper) − Λ_3 − R_{15} branch. The upper HG arises from the crossing of the above mentioned t_{2g}(Ti) branch with the e_g(Ti) Γ_{12} (upper) − Λ_3 − $R_{12'}$ branch.

As a whole, the wide HG found for FeTi around E_F are of the (s(Fe), e_g(Ti)), (s(Fe), t_{2g}(Ti)) and (e_g(Fe), t_{2g}(Ti)) type and evolved from the analogous HG in the BCC transition metal band structure[1]. Therefore, their origin can not be directly related to the existence of order in the alloy.

To summarize, from the qualitative analysis of the band structure we have found in agreement with ref.[11], that the ionicity (arising due to the appearance of new supperlattice NHG around E_F), is the main effect that stabilizes the ordered structure in FeTi.

As to the surface states, FeTi can among others exhibit[21] interesting Shockley surface states in those HG which have been already present in the BCC band structure[1]. Namely, as follows from surface state calculations[22–24] of the (001) face of antiferromagnetic Cr, the introduction of superstructure does not destroy these states.

TABLE IX
Partial wave analysis for two energy branches delimiting the HG in Λ_1 states of FeAl

Point:	Γ	Λ (middle)	R
IR	25′	1	2′
E(Ry)	0·7209	0·6562	0·9056
C(Fe)%	95·614t_{2g}	68·072t_{2g} 6·144s 0·184p	0
C(Al)%	1·611t_{2g}	3·318t_{2g} 3·119s 5·729p	87·384s
IR	1	1	25′
E(Ry)	−0·0619	0·1672	0·4704
C(Fe)%	21·298s	3·117t_{2g} 11·510s 6·409p	52·420t_{2g}
C(Al)%	45·444s	0·374t_{2g} 35·688s 10·632p	26·698p

NHG opened in FeTi due to the superstructure can, in our opinion and contrary to claims in ref.[25], contain only the so-called heteroatomic surface states (see p. 256 of ref.[26] for definition) arising due to the selfconsistency effects[27] and lying close to gap edges. This fact is supported by the experiments[17] on the (011) face of antiferromagnetic Cr which do not show any surface states in NHG or, if they existed, they could only lie very close to the band edges and hence could not be distinguished easily from peaks of van Hove singularities of volume states.

TABLE X

Partial wave analysis for three energy branches around HG in Σ_1 states of FeAl

Point:	Γ	Σ (middle)	M
IR	15	1	1
E(Ry)	1·1236	1·0058	0·9714
C(Fe)%	17·510p	41·644d[a] 10·781s 3·398p	41·781e_g 27·467s
C(Al)%	53·391p	14·297s 8·237p 6·392d	13·246s
IR	25′	1	1
E(Ry)	0·7209	0·6768	0·5602
C(Fe)%	95·614t_{2g}	80·417d 0·640s 0·447p	53·810e_g 12·976s
C(Al)%	1·611t_{2g}	0·816d 0·570s 4·805p	9·137t_{2g}
IR	12	1	5′
E(Ry)	0·5475	0·5496	0·5272
C(Fe)%	77·001e_g	53·683d 3·653s 1·060p	18·852p
C(Al)%	5·982e_g	4·656d 4·937s 9·403p	43·231p

[a] $d = e_g + t_{2g}$.

FeAl Alloy

The band-structure calculations of ref.[8] yield information on several gaps near E_F. Partial wave analysis of those which are HG is given in Tables VII – X.

The data of these Tables show clearly the (sp, e_g) hybridization in Δ_1 and Σ_4 HG. (As a rule, the d character always belongs to Fe atoms, while for the sp character (corresponding to delocalized orbitals), a mixture coming from both Al and Fe is present.) The HG in Δ_1 states corresponds to the (s, e_g) HG in $\bar{\Gamma}_1$ states of the (001) face of β'-CuZn, as given in Table I of ref.[7]. The HG in Σ_4 states in nonhybrizational in β'-CuZn owing to differences in the respective band structures[28].

The (sp, t_{2g}) or (sp, d) hybridization is documented by the Λ_1 and Σ_1 HG. The Λ_1 HG corresponds to the (s, t_{2g}) HG in Table III of ref.[7]. With the Σ_1 HG, the situation is more complicated. The lower Σ_1 branch in Table X changes the character from p to e_g, while the middle one is a hybridized branch of (e_g, t_{2g}) type. Therefore, we expect the presence of other branches at higher energy, which form the upper edge of a (sp, d) HG (*cf.* the highest (p, d) HG in $\bar{\Gamma}_1$ states in Table II of ref.[7]). This is supported *1*) by the existence of the highest Σ_1 branch in Table X with pronounced (sp, e_g) mixing; *2*) by the fact that the wave function of M_3 (upper), situated with energy $E = 0{\cdot}9884$ Ry at the upper edge of the above mentioned HG, contains 65·478% of t_{2g} states (together with 27·453% of s and 1·140% of p character of Al-

TABLE XI

Partial wave analysis for two energy branches delimiting the HG in Λ_3 states of FeAl

Point:	Γ	Λ (middle)	R
IR	25′	3	12
E(Ry)	0·7209	0·6880	0·7789
C(Fe)%	95·614t_{2g}	84·890d[a] 0·807p	98·003e_g
C(Al)%	1·611t_{2g}	3·174d 0·796p	0
IR	12	3	25′
E(Ry)	0·5475	0·5566	0·4704
C(Fe)%	77·001e_g	50·299d 4·833p	52·420t_{2g}
C(Al)%	5·982e_g	3·314d 18·236p	26·698p

[a] $d = e_g + t_{2g}$.

derived states). Summarizing, we have found a pronounced (sp, d) HG in Σ_1 states, which is due to the presence of the (e_g, t_{2g}) hybridization divided into two parts, separated by an (e_g, t_{2g}) hybridized branch.

A careful consideration, based on the partial wave analysis[28] of β'-CuZn, finds an (sp, t_{2g}) HG along Σ_1 at lower energies and hence, there is no strong hybridization with β'-CuZn in the vicinity of E_F. Therefore, the role of (p, d) hybridization for high lying gaps (around 0·6 Ry) appears to have been overestimated in ref.[7]. For the sake of completeness we mention also (see Table XI) the (e_g, t_{2g}) HG in Λ_3 states (*cf.* the HG in $\bar{\Gamma}_3$ states in Table III of ref.[7]). This narrow HG lies below E_F.

To summarize, there are a number of HG around E_F in FeAl with mainly bonding states occupied. This clearly points to an important covalency ingredient in the bonding of this β'-alloy.

The ionicity in the series FeAl, CoAl, NiAl is with great probability determined by narrow *d*-like branches[4,8,12] near E_F (*e.g.* Δ_5, $\Sigma_{2,3}$ and Λ_3 for FeAl) since these lead to a high density of states at E_F and to fulfill selfconsistency requirements, a large charge transfer can arise due to very small changes in the crystal potential. Together with covalency, this charge transfer shares the responsibility for a comparatively large stability of the ordered β'-phase in FeAl.

We do not discuss the surface states of FeAl here since the relevant discussion has been done in ref.[7].

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