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Uichiro Mizutani
Nagoya Industrial Science Research Institute, uichiro@sky.sannet.ne.jp

H. Sato
Aichi University of Education

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U.Mizutani\(^1\) and H.Sato\(^2\)

\(^1\)Nagoya Industrial Science Research Institute, 1-13 Yotsuya-dori, Chikusa-ku, Nagoya, 464-0819, Japan

\(^2\)Aichi University of Education, Kariya-shi, Aichi 448-8542, Japan

uichiro@sky.sanet.ne.jp

Dr.E.Belin-Ferré and I met for the first time at LAM8 conference in Vienna in 1992. We learned that both of us share a common interest in the electronic structure and electron concentration parameter e/a of complex compounds and could produce successive joint papers over 1994 to 2000. After the retirement from Nagoya University in 2005, I have been engaged in studying long-standing e/a issues for transition metal (TM) compounds in collaboration with my co-worker Prof.H.Sato, with the aim at deepening a theoretical insight into the Hume-Rothery electron concentration rule for TM compounds.

Mizutani and Sato have developed the FLAPW-Fourier theory, which is capable of making \textit{ab initio} determination of the number of itinerant electrons per atom, e/a, for elements and compounds, almost regardless of the degree of metallicity, covalency and ionicity involved in the van Arkel-Ketelaar triangle diagram [1-3]. This certainly promises us to pave the way to establish the theoretical basis of the electron theory for any compounds involving TM and/or rare earth elements.

The theory makes a full use of the formalism of the FLAPW (Full-potential Linearized Augmented Plane Wave) electronic structure calculations based on the density functional theory: the j-th wave function in the interstitial region with the energy eigenvalue \(E_j\) at the wave vector \(k_i\) obtained by partitioning the first Brillouin zone into \(N_k\) meshes, is expanded into a Fourier series:

\[
j(r, k_i) = \sum_p \frac{1}{\sqrt{V}} C^j_{k_i+G_p} \exp\{i(k_i + G_p) \cdot r\},
\]

where \(V\) is the volume of the unit cell and \(G_p\) is the reciprocal lattice vector of a given system. The square of the Fourier coefficient \(C^j_{k_i+G_p}\) forms a matrix with the electronic state \(2(k_i + G_p)\) in row and energy eigenvalue \(E^j\) in column. The Fourier coefficients are plotted on the diagram with \(2(k_i + G_p)\) as ordinates and \(E^j\) as abscissa with the choice of \(k_i\) in two ways: one all \(k_i\)‘s in the Brillouin zone and the other \(k_i\)‘s only on its high-symmetry points. The center of gravity energy \(E_{k_i+G_p}^{cg}\) is calculated for each electronic state \(2(k_i + G_p)\) by using the relation:

\[
E_{k_i+G_p}^{cg} = \frac{jE^j(k_i)C^j_{k_i+G_p}^2}{jC^j_{k_i+G_p}^2},
\]
where the sum is taken in the state $|k_i + G_p\rangle$ over first $L$ Fourier coefficients in the descending order in the $j$-th wave function.

The set of $2|k_i + G_p\rangle$, $E_{k_i+G_p}^{CG}$ represents the NFE dispersion relation of itinerant electrons for any crystals including TM elements and their compounds. The $\text{e/a}$ and $\text{e/uc}$, the product of $\text{e/a}$ and the number of atoms per unit cell, can be calculated from $(2k_F)^2$ read off from the intercept of the NFE line with the Fermi level. The critical reciprocal lattice vector $|G_{lc}^2| = 2|\langle k_i + G_p\rangle|_{ZSPS}$ responsible for yielding a gap through the interference phenomenon can be extracted from $E_{k_i+G_p}^{CG}$ closest to the Fermi level.

Figure 1 shows the FLAPW-Fourier spectra for $\alpha$-Fe (cI2) in non-magnetic states, Si (cF8) and the half-Heusler compound NiSnZr (cF12): yellow dots represent the distribution of finite Fourier coefficients at $E^j$ with all possible combinations of $k_i$ and $G_p$. The coloured vertical line segments represent the maximum Fourier coefficients on high-symmetry points and are drawn in proportion to their magnitudes. The coloured circles indicate $E_{k_i+G_p}^{CG}$ on the high-symmetry points. From the intersection of the NFE line with the Fermi level, we obtain $(2k_F)^2 = 1.59 \pm 0.16$, $\text{e/a} = 1.05$, $\text{e/uc} = 2.1$ and $|G_{lc}^2| = 2$ for $\alpha$-Fe. The data for both Si and NiSnZr are incorporated in Figure 1. The possession of common $\text{e/uc} = 32$ and $|G_{lc}^2| = 8$, 11 and 12 for both Si and NiSnZr is consistent with the fulfilment of the interference condition $(2k_F)^2 = |G_{lc}^2|$ or $\text{e/uc} = \frac{1}{3} \left\{ |G_{lc}^2| \right\}^{3/2}$ and explains the origin of the energy gap in terms of the common interference phenomena of itinerant electrons with set of zone planes associated with $|G_{lc}^2| = 8$, 11 and 12 [3].

![FLAPW-Fourier spectra](image)

**Figure 1.** FLAPW-Fourier spectra of (a) $\alpha$-Fe (cI2), (b) Si (cF8) and (c) NiSnZr (cF12) [3].


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