An electronic approach to the prediction of the mechanical properties of magnesium and other light-metal alloys

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Abstract

A quantitative method is reviewed for predicting mechanical properties of magnesium alloys and aluminium alloys. This method is constructed on the basis of molecular orbital calculations of electronic structures. A new parameter, Mk, which is the s-orbital energy level for alloying element in magnesium or aluminium, is introduced and used for the prediction. With this single parameter, the yield strength, the tensile strength and the Vickers hardness are predictable even for commercially available alloys with multiple components.

Riassunto

Viene esaminato un metodo quantitativo per la previsione delle proprietà meccaniche delle leghe di Mg e delle leghe di Al. Il metodo si basa sul calcolo degli orbitali moleculari delle strutture elettroniche. Viene introdotto ed impiegato per la previsione un nuovo parametro Mk, il quale è il livello dell'energia dell'orbitale s dell'elemento alligante di Mg o di Al. Con questo unico parametro si possono predire persino per le leghe in commercio con componenti multiple il carico di snervamento, il carico di rottura e la durezza Vickers.

INTRODUCTION

Magnesium alloys are characteristic of the lowest density among the metallic materials for structural applications. They also have advantage of cutting properties and damping capacity. In response to the strong demand for light-weight components in automotive systems, they have been used widely for the frame of various equipments, the wheel and the head cover of cylinders in automobile engines. Recently their use has been further expanded into the hard disc unit of computers and the carriage of printers. Needless to say, aluminium alloys are most important light-metal alloys used for a variety of industrial fields.

Recently, there has been a potential need for the development of magnesium and aluminium alloys because of their superior properties. However, alloy development has been carried out relying on many trial-and-error experiments, partially due to the lack of theory predicting the mechanical properties of alloys. Despite great progress on the understanding of mechanical properties by dislocation theory, there are still large barriers to the quantitative prediction of alloy strength with the aid of the theory.

Recently, a prediction method has been devised of the mechanical properties for magnesium alloys [1] and aluminium alloys [2]. Both the yield strength and the tensile strength have been predicted quantitatively in terms of an electronic parameter, obtained from the DV - Xα molecular orbital calculation. In the present paper this approach is reviewed, mainly focussing on magnesium alloys.

CALCULATION METHOD

The DV - Xα cluster method is based on the Hartree-Fock-Slater approximation [3]. It provides fairly accurate electronic structures even for a large size of atom cluster system. In case of magnesium, a cluster model used is shown in Fig.1 [4]. In this h.c.p. cluster, a central atom, M, is the alloying element substituted for a magnesium atom, and it is surrounded by 12 first-nearest-neighbour magnesium atoms (called Mg (1)) and by 6 second-nearest-neighbour magnesium atoms (called Mg (2)). The lattice parameters used are a=0.3203 nm and c=0.5199 nm, the same values as in the bulk.

Employing this cluster model, the electronic structures of magnesium containing various alloying elements are calculated, and the s-orbital energy level, Mk, relevant to magnesium is firstly determined theoretically [1]. The values of Mk are given in Table 1 for a variety of alloying elements in magnesium. This Mk is a parameter to show explicitly the alloying behavior of elements in magnesium.

It is stressed here that this Mk parameter is related closely to the electronegativity and the atomic radius of individual alloying element in magnesium [1].

For alloy, the average value is defined as follows,

$$\Delta\overline{Mk} = \sum X_i \left| Mk_i - Mk_{Mg} \right|$$

Here, Mk_i and Mk_{Mg} are the Mk value of the i element and Mg, respectively. X_i is the mole fraction of the i element in the alloy. A difference, $\left| Mk_i - Mk_{Mg} \right|$, may be an indication to show the magnitude of local lattice strain around an alloying element, i, in magnesium, and also an indication to show the magnitude of electronic interactions between i and Mg atoms through the charge transfer between them. Therefore, both the strain effect and electronic effect are reflected in this $\Delta\overline{Mk}$ parameter.

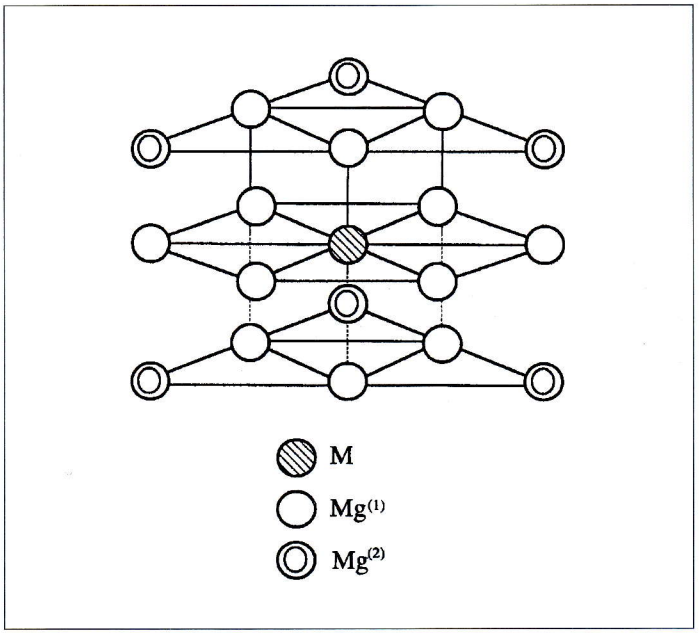

Figure 1: A cluster model, MMg_{18}, used in the calculation

TABLE 1 - Mk values for alloying elements in magnesium

Element	M_k (eV)	Element	M_k (eV)
Li	4.641	Y	4.957
Be	3.891	Zr	4.846
Na	4.664	Nb	4.802
Mg	4.033	Mo	4.787
Al	3.613	Ag	4.354
Si	3.959	Cd	3.999
K	5.059	In	2.737
Ca	4.608	Sn	2.463
Ti	4.341	Sb	2.184
V	4.546	La	6.432
Cr	4.498	Ce	6.400
Mn	4.405	Pr	6.391
Fe	4.393	Nd	6.361
Co	4.352	Sm	6.398
Ni	4.304	Gd	6.404
Cu	4.141	Tb	6.406
Zn	2.727	Dy	6.413
Ga	2.403		
Ge	2.106		

PREDICTION OF MECHANICAL PROPERTIES

1. Magnesium alloys

This $\Delta\overline{Mk}$ parameter is indeed applicable to the quantitative estimation for the mechanical properties of magnesium alloys with multiple components [1]. In Fig.2 the Vickers hardness is plotted against of the $\Delta\overline{Mk}$ for a variety of magnesium alloys. In the figure, the unit, eV, of the $\Delta\overline{Mk}$ is omitted for simplicity. As is evident from Fig.2, the $\Delta\overline{Mk}$ exhibits a good correlation with the hardness. The correlation coefficient is better than 0.94. This means that the hardness is not sensitive to the individual elements in the alloy, but dependent largely on the average compositions weighted by the Mk parameter.

In Fig. 3 the tensile strength is plotted against the $\Delta\overline{Mk}$ for six commercially available alloys. As is evident from this figure, there is a good correlation between the tensile strength and the $\Delta\overline{Mk}$.

In Fig.4 both the tensile strength and the yield strength are plotted against $\Delta\overline{Mk}$ for three cold-chamber die-casting alloys (AE41, AE42 and AZ91) and two hot-chamber die-casting alloys (AM20 and AM50). For cold-chamber die-casting alloys both the strength change linearly with $\Delta\overline{Mk}$. However, for hot-chamber die-casting alloys, the data are too limited to get any conclusion, but the slope of each dotted line seems similar to that of the corresponding solid line. The difference in the respective strength between cold- and hot-chamber die-casting alloys is attributable to the difference in the casting method between them.

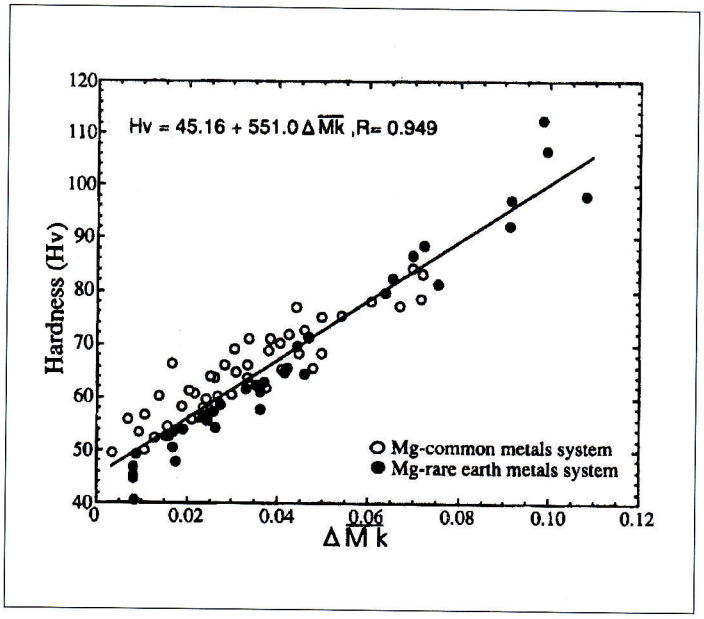

Figure 2: Correlation of the Vickers hardness with $\Delta\overline{Mk}$ for magnesium alloys

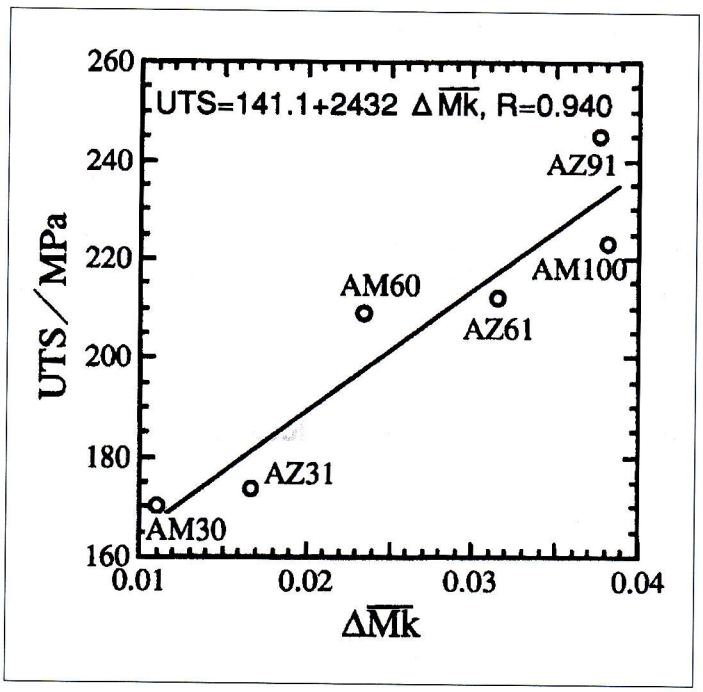

Figure 3: Correlation of the tensile strength with $\Delta\overline{Mk}$ for magnesium alloys

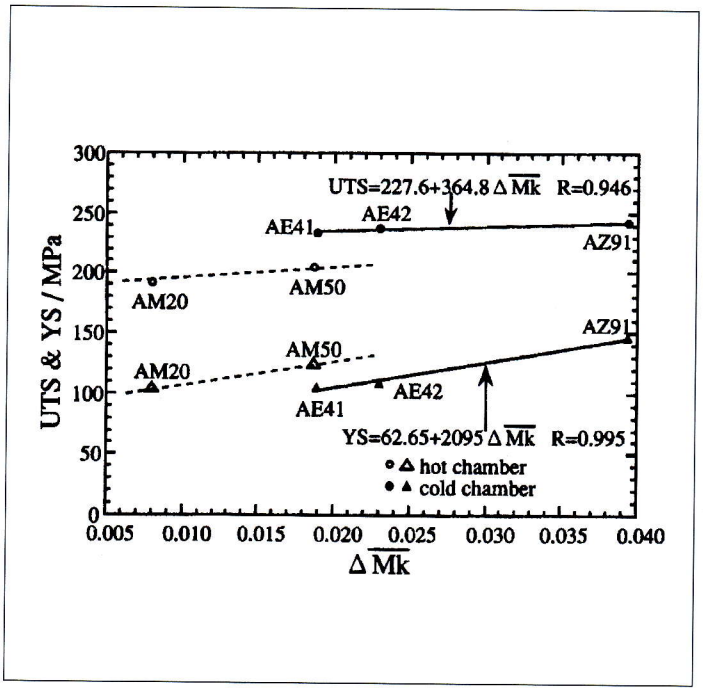

Figure 4: Correlation of the tensile strength (UTS) and the yhield strength (YS) with $\Delta\overline{Mk}$ for magnesium alloys

2. Aluminium alloys

A similar correlation is also seen in aluminium alloys [2]. The values of Mk relevant to aluminium is shown in Table 2 [5].

For example, as shown in Fig.5, the tensile strength of the T6 temper alloys vary almost linearly with $\Delta\overline{Mk}$, and it is less dependent on the alloy types of Al-Cu (2000 series), Al-Mg-Si (6000 series) and Al-Zn-Mg (7000 series), despite the substantial difference in the type of precipitates among them. The yield strengths also vary linearly with $\Delta\overline{Mk}$ as shown in Fig.6. The similar correlation is present in the T4 temper alloys.

Besides these light-metal alloys, this method is applicable to zinc alloys [6].

TABLE 2 - List of the Mk values for alloying element in aluminum

Element	M_k (eV)	Element	M_k (eV)
Li	5.096	Mn	4.443
Be	3.650	Fe	4.328
Na	5.036	Co	4.314
Mg	4.136	Ni	4.248
Al	3.344	Cu	4.037
Si	2.680	Zn	3.290
K	6.196	Ga	3.013
Ca	5.550	Ge	2.614
Sc	5.200	Zr	5.433
Ti	5.009	Nb	5.227
V	4.782	Mo	5.079
Cr	4.601		

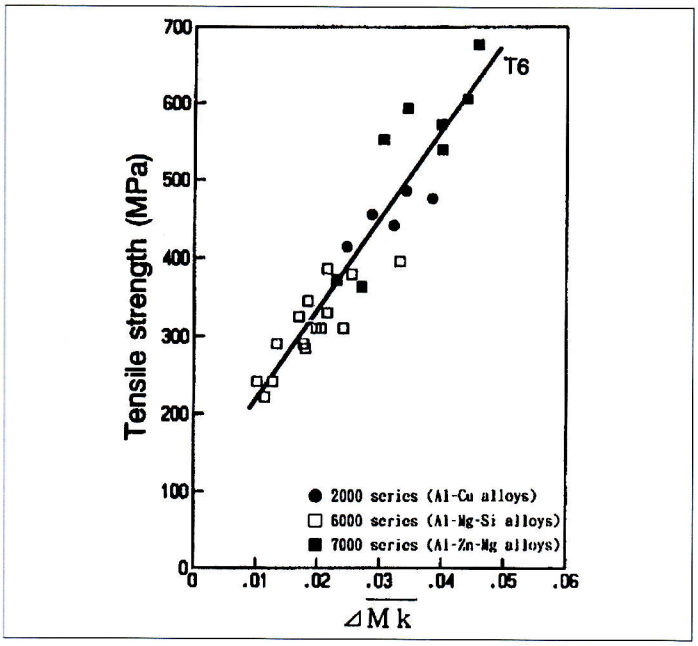

Figure 5: Correlation of the tensile strength with $\Delta\overline{Mk}$ for T6-temper aluminium alloys

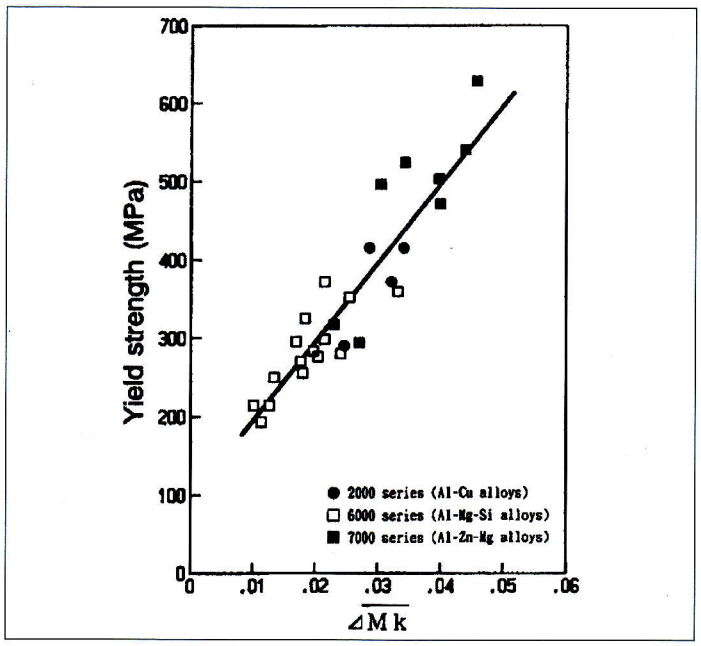

Figure 6: Correlation of the yield strength with $\Delta\overline{Mk}$ for T6-temper aluminium alloys

CONCLUSIONS

A new method is reviewed for predicting the mechanical properties of magnesium and aluminium alloys. The validity of this method is proved firmly by examining the mechanical properties of various alloys with multiple components. This prediction method is very convenient in designing efficiently high performance light-metal alloys.

ACKNOWLEDGMENTS

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