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# Valence electron structure of high manganese steel and its intrinsic property

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Theoretical study on the short-range ordered segregation of alloying elements dissolving in solid solution in C-Me form has made some progress in recent years[1—3], which has already been verified by the electron probe[4], the Mössbauer spectroscopy technique[5], and so on. Based on the empirical electron theory of solids and molecules (EET)[8], and combined with the authors' recent researches, this note deals with the calculations of valence electron structure (VES) of high manganese steel (HMS) with the aim to reveal the intrinsic mechanism of very high austenitic stability, impact toughness, work hardening and impact wear resistance of HMS on the level of its electron structure.

## 1 Valence electron structure of high manganese steel

Austenite in HMS (1.2% C, 12% Mn) is a Fe—Mn—C-alloyed solid solution in which the C atom dissolves in octahedral interstice of FCC $\gamma$-Fe where part of Fe is substituted by Mn. Calculations show that there is averagely one C atom in 3—4, and one Mn atom in 2, austenite cells. Mössbauer spectroscopy tests demonstrate that austenite with C content takes 35%, while that without C takes 65%[5]. The electron probe analysis shows that both C and Mn atoms are distributed heterogeneously in austenite of HMS, and in the microregions where C is abundant, there is abundant Mn and *vice versa*[4, 5].

According to others' finding[6, 7] and the above discussion we can consider that HMS is formed by stacking of cells with and without carbon and those with C—Mn. The principal data of valence electron structure of three kinds of cells are shown in table 1, which were calculated based on EET[6] with $n_A$, the maximum number of covalent electron pair between atoms, of C—C, Fe—Fe and Fe—Mn bonds is within 0.005 3—0.329 9. The calculated results suggest that in all atomic configurations, the bond strengths of C—Mn ($n_A^{C-Mn}=1.2078$)

and C — Fe$^f$ ($n_A^{C-Fe^f}$=0.930 0) are much greater than those of of C — C, Fe — Fe and Fe—Mn. The modern micro-heterogeneity theory has pointed out that when bond between iso-atoms is greater than that between homo-atoms, solute atoms will be distributed in short-range ordered pattern[8] which implies that there exist C — Mn atomic segregations in austenite of HMS.

Table 1 Principal data of VES of 12Mn-1.2C austenite

| Structure unit | Hybrid status of atom | The strongest bond | $n_A$ | Composition of segregation zone |
|---|---|---|---|---|
| Without C | Fe$^c$11, Fe$^f$11 | $D_{n_A}^{Fe^c_e - Fe^f_e}$ | 0.329 9 | Fe$^c$ — Fe$^f$ |
| With C | C6, Fe$^c$13, Fe$^f$14 | $D_{n_A}^{C-Fe^f_e}$ | 0.930 0 | C — Fe$^f$ |
| With C—Mn | C6, Fe$^c$14, Fe$^f$17, Mn11 | $D_{n_A}^{C-Mn}$ | 1 207 8 | C — Mn |

In FCC austenite lattice, only two possible kinds of Fe atoms can be substituted by Mn, i.e the Fe$^c$, which is located on the lattice corner position, and the Fe$^f$, which is located on the lattice face center. In view of the need of carbon for covalent electron and repulsive interaction between neutral (dumping pair) electrons and Mn[3, 4], Mn should substitute Fe$^f$ while it is located on the first neighbouring site of C. We therefore propose a structural model of Fe — Mn — C segregation zone in HMS, showing that the C — Mn atomic segregation zones exist in austenite of HMS where strong C — Fe$^f$ covalent bond leads to C atoms to bound firmly with six Fe$^f$ in the first neighbouring site, and thus a "hard" octahedron is formed. This stronger bond between Mn that substitutes Fe$^f$ and C forms strongly bonded networks —C—Mn—C—Mn—, which further links the octahedron firmly bringing forth the Fe — Mn — C atomic cluster segregation zone (FCSZ) that is strongly linked by strong covalent bonds (see fig. 1). The randomly distributed FCSZ in austenite powerfully affects the motion behavior of atom and dislocation, leading to a series of features of microstructure and properties of austenite in HMS.

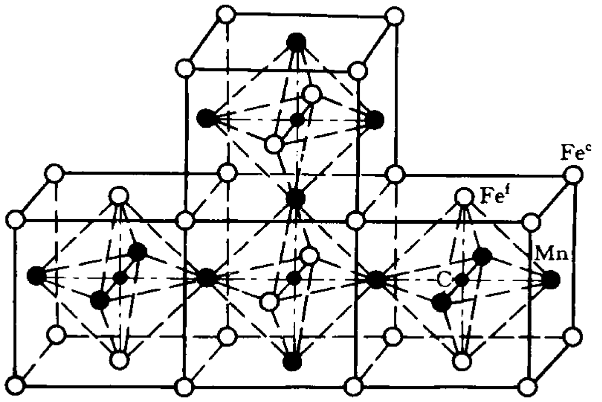

Fig. 1. Atomic arrangement model of FCSZ.

## 2 Intrinsic property and nature of HMS

### 2.1 High stability of austenite

The temperature Ms is below −196℃[4]. The transformation from FCC austenite to BCT marstensite needs lattice reconstruction but the strong networks caused by C — Mn strong bond in the Fe — Mn — C atomic clusters effectively hinder the motion of atoms, making lattice reconstruction difficult and leading to high stability of austenite.

### 2.2 High impact toughness

HMS has a remarkably high impact toughness of up to 150—300 $\mathrm{J/cm}^2$[4]. The toughness of material is essentially its energy absorbing capacity in the process from plastic deformation to fracture[9]. Deformation of HMS needs breaking many C—Mn bonds down and reducing ordering degree of FCSZ, while fracture needs destroying much more numbers of C—Mn bonds, which will absorb more energy, showing high toughness macroscopically.

### 2.3 High work hardening ability (WHA)

HMS has an unusual high WHA with work hardening index above 0.45[4]. In austenite of HMS, the C atom is located at the center of octahedral interstice of lattice, and also located between two neighbouring slip planes (111). Mn, which substitutes Fe, is located at the face center and also located on two slip planes (see fig. 2). When slip occurs it necessarily breaks down many strong C—Mn bonds and sub-strong C—$\mathrm{Fe}^{\mathrm{f}}$ bonds, so FCSZ will have a potent resistance against the start of slip system. This was verified by absence of obvious yielding point during tensile deformation and with high WHA behavior at the initial stage of plastic deformation for HMS[4].

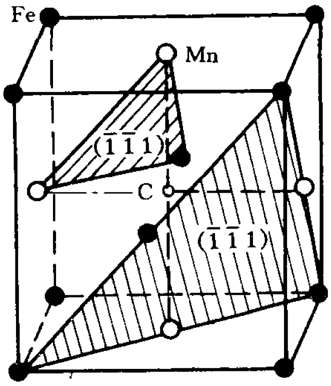

Fig. 2. Model of C—Mn-involved cells.

During deformation, when moving dislocation meets FCSZ which is distributed randomly in austenitic matrix, C atoms will be trapped in the central portion of dislocation. As Mn and $\mathrm{Fe}^{\mathrm{f}}$ atoms strongly tie up with C atoms, the motion of C atoms following dislocations will thus be limited, thus retarding the moving of dislocations. On the other hand, when moving dislocations pass over FCSZ, not only many strong C—Mn bonds become broken, but also the atoms lying on both sides of the slip plane will reconstruct and the short-range ordering degree will be reduced. This must deplete energy causing strengthening effect on HMS during its deformation.

Relationship between the increase of flow stress $\Delta\tau$ caused by FCSZ and $M_{\mathrm{C}}$ and $M_{\mathrm{Mn}}$, the mole fractions of C and Mn, respectively, as well as $n_{\mathrm{A}}$ can be expressed as

$$\Delta\tau = KM_{\mathrm{C}}M_{\mathrm{Mn}}n_{\mathrm{A}}a_1/a^3,$$

where $K$ is the ratio coefficient; $a_1$ the parameter of the first neighbouring short-range order, and $a$ is the lattice parameter.

### 2.4 Excellent impact wear resistance

In HMS, unusual high WHA caused by FCSZ which retards the start of slip system and the movement of dislocations leads to a high hardness of wearing surface, thus reducing the cut and deformation wear. Strong network —C—Mn—C—Mn— and high toughness caused by it can effectively retard the emerging of crackle and peeling off of matrix material, thereby reducing wear caused by fatigue stripping. As a result, HMS has an excellent impact abrasion resistance.

## 3 Concluding remarks

From calculations of valence electron structure and many experimental results, it is suggested that there exist —C—Mn—C—Mn— strong-bond networks and FCSZs in HMS. The great influence of FCSZ on moving behavior of atoms and dislocations is the intrinsic mechanism for HMS with very high austenitic stability, impact toughness, WHA and. impact wear resistance.

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