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Computer aided design of free-machinability prehardened mold steel for plastic①

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Abstract: In order to improve the machinability but not to impair other properties of the prehardened mold steel for plastic, the composition was designed by application of Thermo-Calc software package to regulate the type of non-metallic inclusion formed in the steel. The regulated non-metallic inclusion type was also observed by SEM and EDX. Then the machinability assessment of the steel with designed composition under different conditions was studied by the measurement of tool wear amount and cutting force. The results show that the composition of free cutting elements adding to mold steel for plastic can be optimized to obtain proper type of non-metallic inclusion in the aid of Thermo-Calc, compared with the large volume fraction of soft inclusion which is needed for promoting ductile fracture at low cutting speeds, the proper type of inclusion at high cutting speeds is glassy oxide inclusion. All those can be obtained in the present work.

Key words: prehardened mold steel for plastic; machinability; Thermo-Calc software package; non-metallic inclusion
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1 INTRODUCTION

Prehardened mould steel for plastic with 36-42HRC is difficult to machine and good machinability of such mould steel is requested as usual. A familiar way to meet the requirement is to add free-cutting elements, such as sulphur and calcium. It is shown that modified effect of calcium treatment on non-metallic inclusion precipitated in steel can be optimal if the ratio between calcium and sulphur is fixed as about 0.7[1] or 3[2] or 0.07-0.12[3] determined by experiments.

However, it is not always the case for all kinds of steels. Generally in order to obtain the proper type of non-metallic inclusion for calcium treated steel, the quantity and type of free cutting elements can be regulated by thermodynamic computation. During calcium treatment of aluminum killed steels, the type of oxide and sulphide formed at given temperature can be predicted by computing the thermodynamic behavior of the Fe-Al-Ca-O-S system[4-6]. It is obvious that this kind of computation is too simple for the practical process of non-metallic inclusion formed in steel, considering complex thermodynamic equilibrium relationship among multi-components, which should be more than five components, and multi-phase systems. In addition, the reliability of relevant thermodynamic parameters is vital to application of thermodynamic computation. So an effective tool with powerful computational function and reliable database are needed to make the method applicable and convenient.

Thermo-Calc, a commercial software package for calculating the phase equilibrium from a broad database, offers an appropriate access for the materials design and reduces the times of experiments[7, 8]. The SLAG database of the commercial software package from IRSID for Fe-containing slag can be used for predicting the composition of non-metallic inclusion formed during steel-making with a specific multiphase equilibrium[9-11].

In this article, aided by Thermo-Calc software package, it can be predicted that the possible type of free cutting phase forms in the prehardened mold steel for plastic. Then the contents of sulphur and calcium can be precisely regulated in order to effectively improve the machinability of steel.

2 THEORETICAL MODEL AND COMPUTATIONAL MODELLING

The SLAG database from IRSID for Fe-containing slag consists of data for the liquid slag and condensed oxides for the Al_2O_3-CaO-Fe_2O_3-FeO-MgO-SiO_2 system. The liquid slag is described with Gaye-model in the database. Gaye et

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al[12] investigated a liquid slag mixture of m oxides $((M_i)_{u_i}O_{v_i}$, $i = 1, 2, \cdots, m)$ including two kinds of sub-lattice. One is an anionic sub-lattice filled with oxygen ions and the other is cationic sub-lattice filled with the cations in the decreasing order of their charge (e. g $Si^{4+} \cdots Ca^{2+} \cdots$). And the structure of the melt is described in term of symmetric (i-O-i) and asymmetric (i-O-j) cells, in numbers R_{ii}, $\cdots$, $2R_{ij}$, $\cdots$. The energy parameters consist of parameters for asymmetric cells formation, and parameters of interaction between cells. This simplified melt structure makes it possible to describe the multi-component system in terms of only a few binary parameters. Because the formation of melt can be thought as the result of the following bond response:

$$(i\text{-O-}i) + (j\text{-O-}j) = 2(i\text{-O-}j) \quad (1)$$

Then the expression for the mixing free energy G^M of the melt can be derived by statistic thermodynamic method and thermodynamic parameters of all oxide components can be determined:

$$G^M = 2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left[R_{ij}W_{ij} + R_{ii}\frac{v_i x_i}{D_1}E_{ij}\right] - RT\sum_{i=1}^{m-1}\frac{u_i}{v_i}\left[D_i\ln\left(\frac{D_i}{v_i x_i}\right) - D_{i+1}\ln\left(\frac{D_{i+1}}{v_i x_i}\right)\right] - RT\sum_{i=1}^{m}\sum_{j=1}^{m}\left[R_{ij}^*\ln R_{ij}^* - R_{ij}\ln R_{ij}\right] \quad (2)$$

$$\sum_{j=1}^{m}R_{ij} = v_i x_i \quad (3)$$

$$R_{ii}\cdot R_{jj} - \frac{R_{ij}^2}{P_{ij}^2} = 0$$

$$(j = i+1, i+2, \cdots, i+m) \quad (4)$$

$$D_i = \sum_{k=i}^{m}v_k x_k \quad (5)$$

$$R_{ij}^* = (v_i v_j x_i x_j)/D_1 \quad (6)$$

$$P_{ij} = \begin{cases} 1 & \text{if } j = i \\ \exp(Q_i)\exp(Q_j)\exp\left(-\frac{W_{ij}}{RT}\right) & \text{if } j \neq i \end{cases} \quad (7)$$

$$Q_i = \sum_{k=i+1}^{m}(v_k x_k/D_1)(E_{ik}/RT) \quad (8)$$

$$Q_j = \sum_{k=j+1}^{m}(v_k x_k/D_1)(E_{jk}/RT) \quad (9)$$

where m is number of oxides $(M_i)_{u_i}O_{v_i}$; u_i, v_i are stoichiometric indexes of oxides; x_i is molar fractions of oxides; R_{ii}, $2R_{ij}$ are numbers of i-O-i, i-O-j cells; W_{ij} is energy parameters for asymmetric cells formation; E_{ij} is energy parameters for cells interactions; R_{ij}^* is fraction of i-O-j cells for a random distribution of cations on their sublattice.

The model was incorporated in various multi-phase equilibrium calculation models for the description and monitoring of metal-gas-slag treatments and then the database based on it can be applied to estimate the type and amounts of non-metallic inclusion at different stages in the production of steel[13-16].

In this study, the SLAG database is first applied to estimate the effect of calcium, aluminum and sulphur content on non-metallic inclusion precipitate in mold steel for plastic with matrix composition of 0.4% C, 1.37% Mn, 1.77% Cr, 0.9% Ni, 0.2% Mo, 0.3% Si (mass fraction). This kind of effect is quantitatively analyzed by means of computational procedure in Thermo-Calc software. While performing analysis, the composition of the steel as well as the temperature considered are input into the computer as a macrofile. Take addition of 0.02% or 0.04% S for example, when the oxygen content is fixed as 4.0×10^{-5}, it can be calculated that $Ca_2O_2\cdot SiO_2$, CaS, calcium aluminates, including $CaO\cdot 2Al_2O_3$, $CaO\cdot 6Al_2O_3$ and liquid $2CaO\cdot Al_2O_3\cdot SiO_2$ (C2AS) etc form in different composition ranges, as shown in Fig. 1, respectively.

It can be seen that between 2.17×10^{-5} and 4.0×10^{-5} of calcium content, free cutting phase C2AS can be precipitated in steel with 0.02% of sulphur and 1.5×10^{-4} aluminum; then if 0.04%

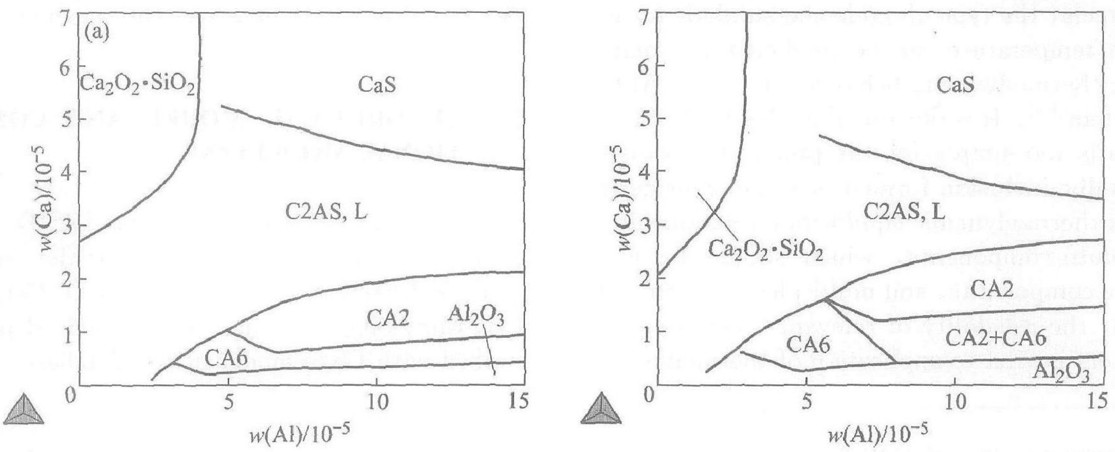

Fig. 1 Effect of Ca and Al content on non-metallic inclusion precipitated in steel for content of S 0.02% (a) and 0.04% (b) at 1550 ℃

of S is added, calcium content is between 2.72×10^{-5} and 3.49×10^{-5}. The composition range is so small that it makes regulation difficult.

As is well known, calcium aluminates precipitate before solidification easily form cluster and then big chunk of inclusion, even form defects in steel during solidification. In addition, the formation of solid calcium sulphide inclusion not only produces the aggregation of calcium aluminate but also hinders the formation of free cutting phase MnS during solidification. Thus, if the free cutting element contents are not controlled, the performance of calcium treated steel may be decreased resulting from the formation of harmful inclusion. On the contrary, glassy oxide inclusion C2AS benefits to the machinability of steel but almost does not impair the mechanical properties[17-19]. According to the calculated result if sulphur and calcium contents are regulated to proper range under given condition, free cutting phase can be obtained, which will be testified by following experiments.

3 EXPERIMENTAL AND RESULTS

The experimental materials are melted in a middle frequency induction furnace. The mass of each ingot is 30 kg. The chemical compositions of steel tested are given in Table 1. The ingots are hot-forged into bar 85 mm in diameter and 300 mm in length. These samples are quenched and tempered to a hardness of 41HRC.

Specimens of 12 mm × 12 mm × 12 mm are cut from the cast ingot for energy dispersive system analysis of inclusion, the result is shown in Fig. 2. A lathe with a variable spindle speed capability is used for turning tests. In the experiment of tool wear test at low cutting speed, the cut depth and feed rate are fixed as 1.5 mm and 0.1 mm/r, respectively, whilst the cutting speed is variable in the range from 15 m/min to 32 m/min; then at high cutting speed, the cutting speed is variable in the range from 150 m/min to 230 m/min. In the experiment of cutting force test, the feed rate is fixed as $f = 0.1$ mm/r and the cutting speeds are fixed as $v = 40$ m/min and $v = 170$ m/min respectively, whilst the cut depth is variable in the range from 0.5 mm to 3 mm. The principle cutting force F_Z is measured by a three-component piezoelectric force dynamometer. The flank wear of the tool at different times are measured by using a tool maker's microscope with precision of 0.01 mm. The flank wear of the tools whilst machining experimental steel are shown in Fig. 3(a) and the principle cutting forces when machining the steels tested at different cut depth are shown in Fig. 3(b). Then the rake surface of tool is observed by SEM and EDX after cutting the No. 2 steel for 5 min using the cutting speed at 230 m/min, the results are shown in Figs. 4(a) and (b).

4 DISCUSSION

As shown in Fig. 2(c), alumina inclusion with 2-3 μm size is found in untreated steel. In Figs. 2(a) and (b) it can be seen that the main types of inclusion in No. 2 steel are C2AS and (Mn, Ca)S plus minuscule calcium aluminate complex inclusion respectively. The experimental results agree with the calculation results, that is to say, the formation of harmful inclusion can be avoided and C2AS free cutting phase can be precipitated in steel with addition of 0.02% of S and 3.7×10^{-5} calcium in given condition.

During the cutting process the wear and failure mechanisms of tools are very complex. The mechanism and process, including plastic deformation under compressive stress, diffusion wear, attrition wear and abrasive wear, etc, appear to be the main ways in which carbide tools are worn or change shape so that they no longer cut effectively[20].

The former two failure modes based on deformation and diffusion are temperature dependent and come into play at high cutting speeds[21, 22]. As for diffusion wear, metal and carbon atoms of the tool material diffuse into the work material that is seized to the rack face surface, these atoms are then carried away in the body chip. Under lower cutting speed condition, temperature is low, the abrasive wear and attrition wear dominate. Generally the abrasive of rake and flank surface by hard particles, such as alumina existed in the steel, will play an important role in the wear of tools.

In the machinability experiments, as shown in Fig. 3, it is obvious that tool wear and principle cutting force whilst machining the No. 1 steel are all much greater than those whilst machining No. 2 steel at low or high cutting speeds. In addition after cutting the No. 2 steel for 5 min using the cutting speed at 230 m/min, the C2AS lubricating lay-

Table 1 Chemical composition of steel tested (mass fraction, %)

No.	C	Mn	P	S	Si	Ni	Cr	Mo	V	Al_s	Al_t	O	Ca
1	0.40	1.36	0.019	0.008	0.30	0.90	1.78	0.20	0.10	.015	.025	39	–
2	0.40	1.37	0.019	0.021	0.31	0.91	1.77	0.20	0.11	0.014	0.021	37	37

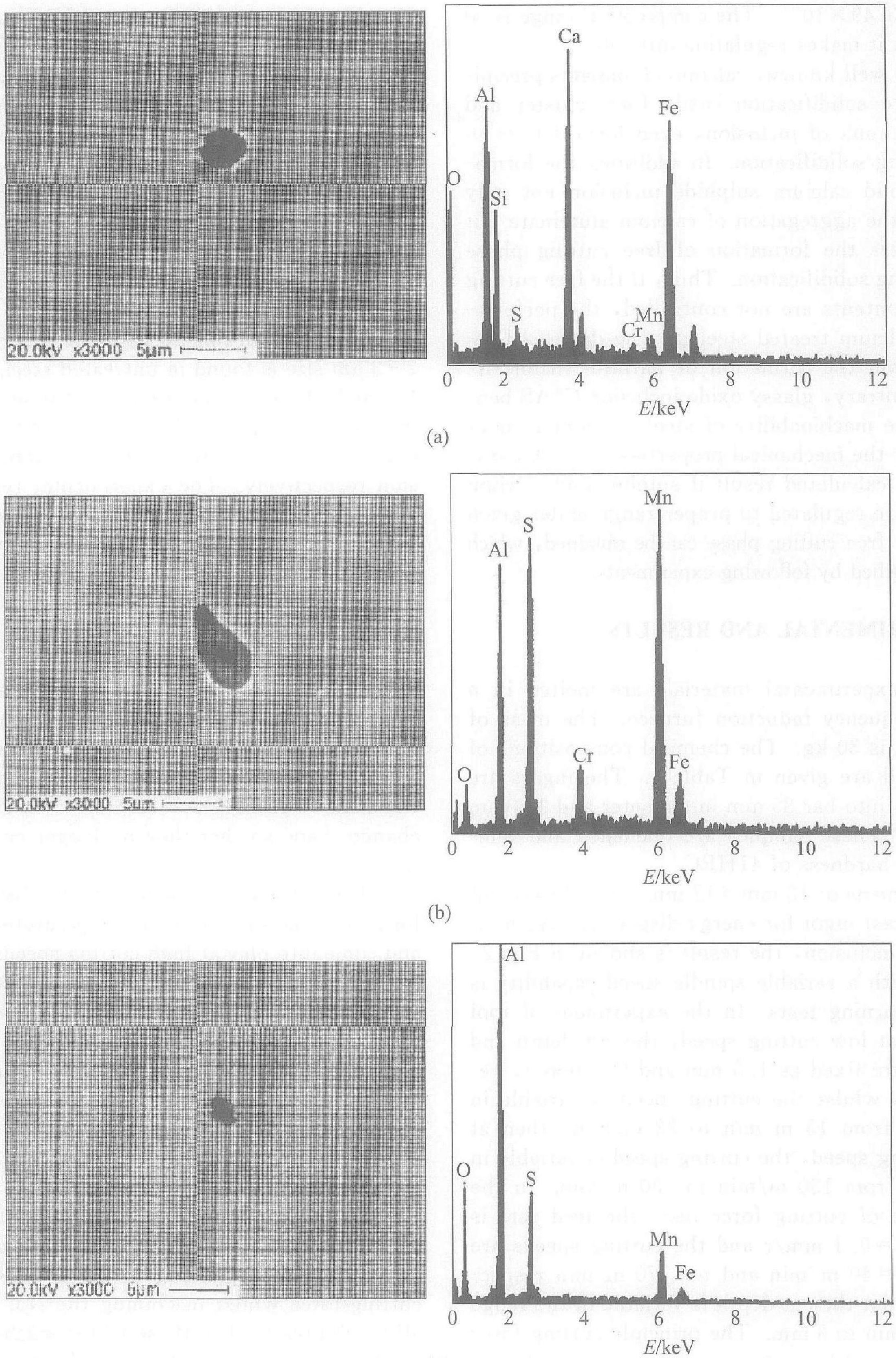

Fig. 2 Morphologies of inclusion in steel and their composition analysis
(a), (b) —No. 2 steel; (c) —No. 1 steel

er is observed at the rake face of tool.

At low cutting speed, the tribological condition at the tool/chip interface is sliding, physical wear processes dominate[23]. (Mn, Ca)S plus calcium aluminates complex inclusion dispersed in steel No. 2 can improve the machinability. Because the incompatibility of deformation between such soft inclusions and the steel matrix promotes damage events leading to ductile fracture, i. e. void nucleation, void growth and void coalescence. In contrast, the wear of tool for cutting No. 1, which is

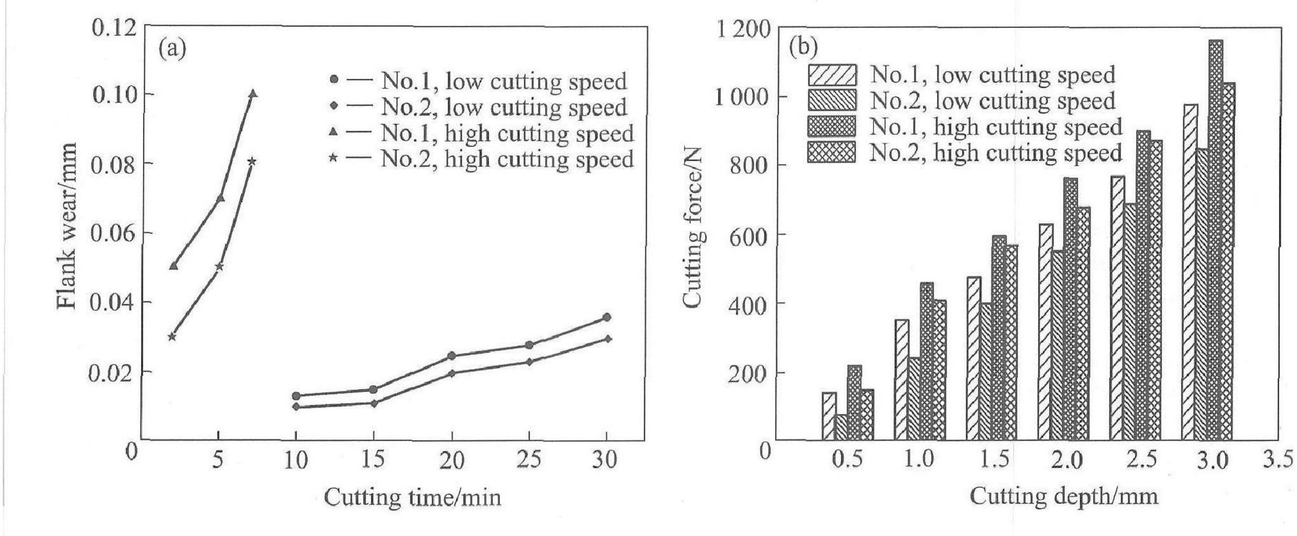

Fig. 3 Results of cutting test for experimental steels
(a) —Flank wear of tool; (b) —Principle cutting force

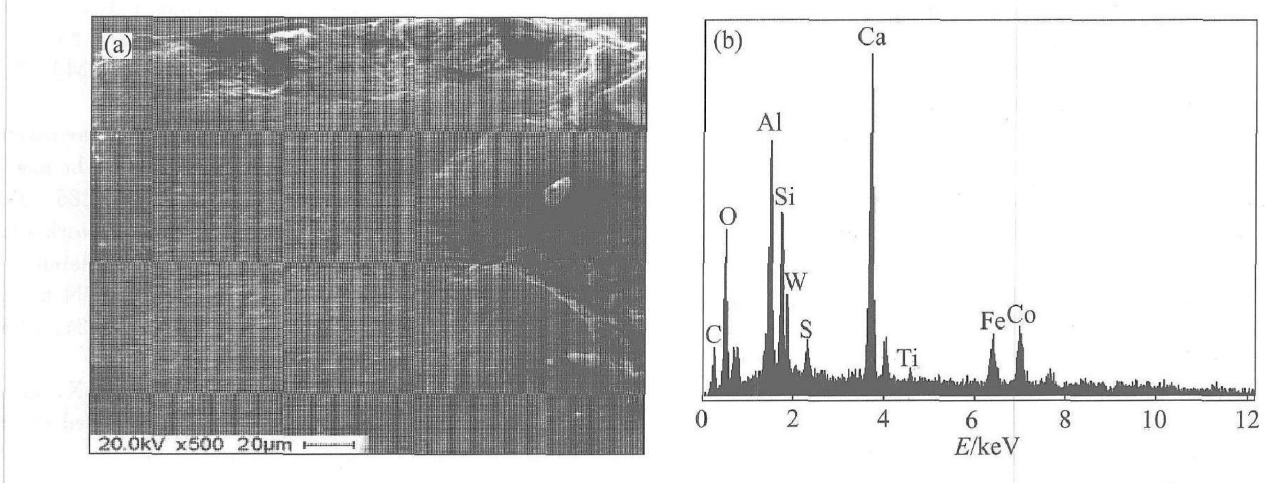

Fig. 4 Observation of tool rake at high cutting speed of morphology(a) and composition analysis(b)

the untreated steel whose microstructure and mechanical performance similar to No. 2 steel, is accelerated by the abrasive action of very hard rigid alumina inclusion. At high cutting speed the tool diffusion wear is the dominant failure mode in machining steel. It is shown that in the condition of cutting speed between 100 m/min and 250 m/min, feeding rate between 0.07 mm/r and 0.2 mm/r, the cutting temperature is about 700 - 900 ℃, that is equal to the turning point of viscosity-temperature relation curve for CaO-Al_2O_3-SiO_2 inclusion[24], which means the viscosity of glassy oxide inclusion located in the interface of tool/chip, is markedly decreased and forms the protective layer on the tool under high press, high friction and high temperature. This layer not only reduces the friction wear but also suppresses the diffusion wear, because alloy elements in tool material diffuse into chips are inhibited and dynamic diffusional process effectively change into quasi-static state diffusion mode. So it can be concluded the machinability of No. 2 steel is better than No. 1 steel due to the formation of free cutting phase.

5 CONCLUSIONS

1) Free-machinability prehardened mold steel for plastic can be designed by Thermo-Calc software package. Free cutting phase can be precipitated in steel by the regulation of sulphur and calcium contents at the simulated composition range.

2) The formation of (Mn, Ca)S plus calcium aluminates complex inclusion and C2AS benefits to improve the machinability of prehardened mold steel for plastic at low or high cutting speed.

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