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# Revisiting the formation mechanism of intragranular $\kappa$ -carbide in austenite of a Fe-Mn-Al-Cr-C low-density steel

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## Abstract

It was usually believed that the formation of intragranular  $\kappa$ -carbide in  $\gamma$ -austenite was attributed to spinodal decomposition followed by ordering reaction. In this work, near-atomic scale characterization of an austenite-based Fe-20Mn-9Al-3Cr-1.2C (wt. %) low-density steel, using (high-resolution) scanning transmission electron microscopy and atomic probe tomography, reveals that the initially-formed  $\kappa$ -carbides (2-3 nm in particle size) are featured with an ordered L'1<sub>2</sub> structure but without detectable chemical partitioning. Further, the Gibbs energy of the FCC phase obtained by thermodynamic calculations always shows a positive curvature (i.e.  $\frac{d^2G}{dx^2} < 0$ ) with the variable contents of Al and C in the temperature range 400-800 °C. Both the results demonstrate that the ordered nuclei of  $\kappa$ -carbide can form directly in the disordered  $\gamma$ -austenite rather than through the well-known spinodal decomposition-ordering mechanism. The extremely low nucleation barrier is due to the similar lattice structure, same composition and complete coherency between the  $\gamma$ -austenite matrix and  $\kappa$ -carbides.

**Keywords:** Low-density steel,  $\kappa$ -carbide, Spinodal decomposition, Atom probe tomography (APT), Thermodynamic calculation.

Precipitation strengthening promoted by nano-scale  $\kappa$ -carbides in austenite-based

Fe-Mn-Al-C low-density steels has received much attention since such shearable and coherent precipitates within the  $\gamma$ -austenite matrix significantly enhance strength without sacrificing too much elongation [1-6]. The ideal stoichiometry of intragranular  $\kappa$ -carbide is  $(\text{Fe, Mn})_3\text{AlC}$ , and it has a perovskite crystal structure designated as  $\text{E2}_1$  in the Strukturbericht classification [1]. Based on observations of electron diffraction patterns and calculations of structure factors, an elemental site-occupancy in the  $\kappa$ -carbide was summarized as that Fe and Mn atoms were located at face center positions, Al atoms at corner positions, and C atom at body center octahedral ( $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ ) interstitial position of this structure [1, 7, 8]. It was reported that the  $\kappa$ -carbide could initially form at the solid solution state [4, 9-11], and its coarsening occurred during isothermal aging treatments in the temperature range 450-600 °C [1, 12-14].

It has long been believed that in most austenite matrix alloys, the formation of intragranular  $\kappa$ -carbide is through spinodal decomposition and following ordering reaction [1, 15, 16]. Its formation sequence is generally described as follows [1]: a spinodal decomposition divides high temperature  $\gamma$ -austenite into the solute-lean (C and/or Al) phase  $\gamma'$  and the solute-rich phase  $\gamma''$ ; then the solute-rich phase  $\gamma''$  transforms into the ordered  $\text{L1}_2$  phase, in which Al and Fe/Mn atoms are located at corner and face center sites, respectively; finally, the  $\kappa$ -carbide with  $\text{E2}_1$  structure forms by further ordering of C atoms. Usually, the non-stoichiometric  $\kappa$ -carbide  $((\text{Fe, Mn})_3\text{AlC}_x)$  is observed being referred as  $\text{L}'1_2$  ordered phase.

In the early years, conventional transmission electron microscopy (TEM) and X-ray diffraction (XRD) were used as the main tools to provide experimental evidence supporting the spinodal decomposition-ordering mechanism by observing the modulated structure [17], diffuse satellites around the (020) diffraction spots in electron diffraction patterns and XRD sideband peaks around the (200) reflections [16, 18]. Over recent years, the composition uncertainty of  $\kappa$ -carbide was quantitatively resolved at near-atomic scale by atom probe tomography (APT) [4, 7, 12]. The concentration profiles with sinusoidal curves across the  $\gamma$ -austenite matrix and developed  $\kappa$ -carbide were found to confirm the occurrence of spinodal decomposition during  $\kappa$ -carbide precipitation [12, 19].

However, very recent TEM and APT results obtained in a Fe-30Mn-9Al-1.2C (wt. %) lightweight steel surprisingly indicated that the formation of an ordered structure was earlier than chemical partitioning of any solute elements during the early stage of  $\kappa$ -carbide precipitation [4]. This observation obviously challenged the general understanding of the  $\kappa$ -carbide formation process. In fact, the study of  $\kappa$ -carbide mainly focused on the coarsened  $\kappa$ -carbide at the aged states where both  $\text{L}'1_2$  ordered structure and chemical partitioning were observed. Comparatively, the

study of the  $\kappa$ -carbide formation at the initial stage is still very limited due to tiny size of  $\kappa$ -carbide in the range of a few nanometers and complete coherency with  $\gamma$ -austenite. Therefore, the understanding of  $\kappa$ -carbide formation process at the initial stage has still been insufficient. The objective of this work is to revisit the formation mechanism of  $\kappa$ -carbide in an austenite-based Fe-20Mn-9Al-3Cr-1.2C (wt. %) low-density steel at near-atomic scale by probe-corrected (high-resolution) scanning TEM ((HR)STEM), APT and thermodynamic calculation.

As detailed in our previous works [9, 20], the steel sample was prepared by centrifugal casting under near-rapid solidification in an argon atmosphere. Molten metal was poured directly into a copper mold and solidified at a cooling rate higher than  $10^3$  K/s [21]. Isothermal aging was carried out under vacuum at 600 °C for 9 h, followed by furnace cooling. Chemical composition of the as-cast steel, measured by an inductively coupled plasma-atomic emission spectrometry (ICP-AES) and a carbon-sulfur analyzer (CS2800), was Mn 19.70 wt. %, Al 8.86 wt. %, Cr 2.90 wt. %, C 1.21 wt. % and Fe balance.

TEM examination was carried out using a FEI Tecnai G2-20 twin and a Thermofisher Titan Themis 300 microscopes, operated at 200 and 300 kV, respectively. The latter was equipped with a probe aberration corrector allowing to acquire (HR)STEM images. The probe size was set to 0.1 nm with a convergence semi-angle of 22.5 mrad. Collection angle of the high-angle annular dark-field (HAADF) imaging detector was in the range 80-150 mrad. TEM specimens were prepared by twin-jet electrolytic polishing at -30 °C and 30 V, with a mixed solution of 10 % perchloric acid and 90 % alcohol. Dr. probe software was used for atomic-scale HAADF image simulation [22]. Standard two-step electro-polishing was used to prepare needle-like specimens for APT using a local electrode atom probe instrument (CAMECA LEAP 4000 XHR), in laser-pulsing mode with a repetition rate of 200 kHz, a pulse fraction of 15 %, and a specimen temperature of 50 K. Post-treatment of APT data was done using IVAS 3.6.8 software (CAMECA software suite). The peak decomposition algorithm in IVAS was used to resolve the peak overlaps among Fe, Al and Cr at 27 Da in mass spectrum, which has been proven to significantly improve counting statistics [23, 24].

Thermodynamic calculations were performed by Thermo-Calc software using previously-created thermodynamic database of low-density steels [25-29]. Partitioning model based on the Compound Energy Formalism (CEF) was employed to describe disordered and ordered forms (such as  $L1_2$  and  $L1_0$ ) of the FCC phase in the database and the detailed calculation process was given in [Supplementary](#).

The DF-TEM images (in Fig. 1 (a) and (d)) show that the homogeneously

dispersed  $\kappa$ -carbide precipitates are present at the as-cast and aged states, and have the average sizes of around 3 and 10 nm, respectively. Being consistent with the previous results [1], the selected area diffraction patterns (SADPs, insets in Fig. 1 (a) and (d)) show that the  $\kappa$ -carbides have a cube-on-cube orientation relationship with the  $\gamma$ -austenite:  $[100]_{\kappa} // [100]_{\gamma}$  and  $(100)_{\kappa} // (100)_{\gamma}$ . By measuring the  $\{100\}$  and  $\{110\}$  superlattice reflection intensity in SADP shown in Fig. 1 (a) and (d), the intensity ratios of  $I_{(011)}/I_{(001)}$  in the as-cast and aged samples are 0.52 and 0.25, respectively. This suggests that the ordering of C atoms in the body-center octahedral sites is gradually improved with the growth of  $\kappa$ -carbides. It was reported that the intensity of the  $\{100\}$  superlattice spots is higher than the  $\{110\}$  ones in  $L'1_2$  structure [17, 30, 31]. Since theoretically the intensity of the superlattice reflections is proportional to square of the structure factor ( $F_{hkl}$ ,  $h$ ,  $k$  and  $l$  are the Miller indices), the  $L'1_2$  structure with partially C ordering can be distinguished [32]. Contrasts in an HAADF image is proportional to  $Z^{-1.7-2}$  [33], meaning that the bright contrast indicates Cr- ( $Z=24$ ), Mn- ( $Z=25$ ) and/or Fe-rich ( $Z=26$ ) atomic columns, while dark contrast represents Al- ( $Z=13$ ) and/or C-rich ( $Z=6$ ) atomic columns in this case. Thus, the individual  $\kappa$ -carbide precipitates can be identified using FFT patterns shown in Fig. 1 (b) and (e), which have the fully coherent interface with the  $\gamma$ -austenite matrix and no interfacial misfit dislocation is visible. Although the exact atomic occupations of Cr and Mn are unknown, the contrasts of the  $\kappa$ -carbides approximately correspond to those of the simulation results using the  $E2_1$  structural model shown in Figs. 1 (c) and (f).

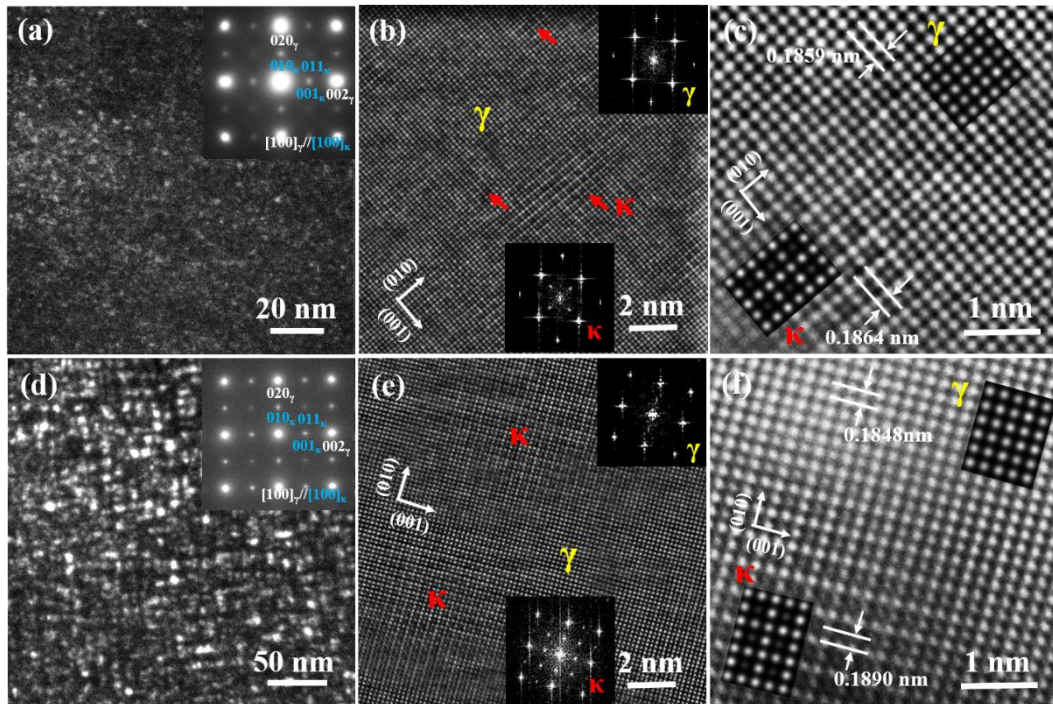


Fig. 1 (HR)(S)TEM characterization of the as-cast (a-c) and aged steels (d-f): (a) and (d) are



dark-field (DF) TEM images, insets are corresponding SADP of  $[100]_{\gamma}$  zone-axis; (b) and (e) are filtered HRSTEM-HAADF images along  $[100]_{\gamma}$  zone axis, insets are corresponding *fast Fourier transform* (FFT) patterns of  $\gamma$ -austenite and  $\kappa$ -carbide; (c) and (f) are zoom-in images of (b) and (e) respectively, overlapped images are simulated HRSTEM-HAADF images using  $\kappa$ -carbide ( $E2_1$   $Fe_3AlC$ ) and  $\gamma$ -austenite (FCC Fe) structure models.

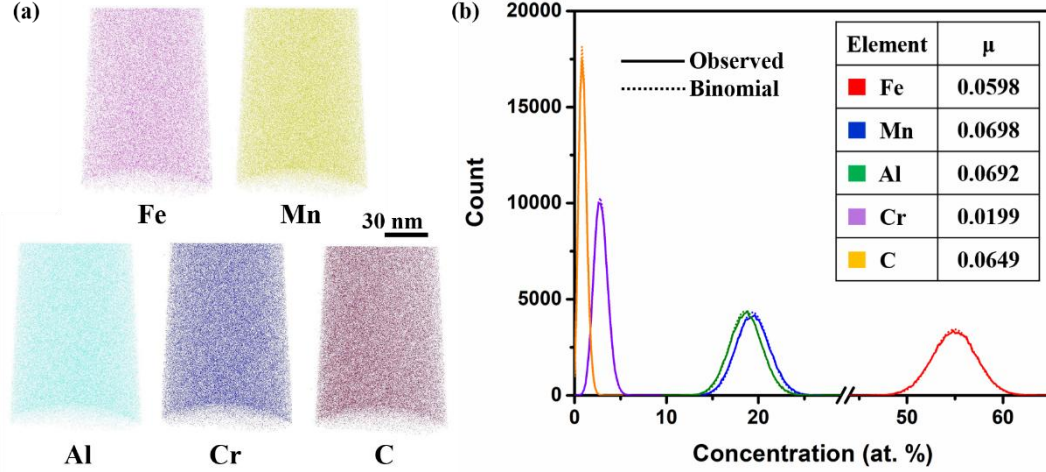


Fig. 2 APT characterization of  $\gamma$ -austenite in the as-cast steel: (a) Fe, Mn, Al, Cr and C elemental maps; (b) frequency distribution analysis obtained by comparing the observed experimental results and the binomial simulation, and the values of normalized homogenization parameter  $\mu$  are listed in the inserted table in (b).

The APT result in Fig. 2 (a) shows that the distributions of all the five solute elements (Fe, Mn, Al, C and Cr) are visibly uniform in  $\gamma$ -austenite of the as-cast steel. According to the TEM-DF image shown in Fig. 1 (a), the density of the  $\kappa$ -carbides with a size of 3 nm is almost  $3/100 \text{ nm}^2$ . It is estimated to have at least 294 observable  $\kappa$ -carbide particles in the 2-dimensional surface of the APT-reconstructed map if chemical ordering exists. However, no chemical partitioning caused by the formation of tiny  $\kappa$ -carbides (confirmed by TEM in Fig. 1 (a-c)) is detected. As shown in Fig. 2 (b), the observed data (solid line) fit with the binomial random distribution model (dotted line), and the values of the normalized homogenization parameter  $\mu$  are all close to 0, indicating the random distribution of all the elements at the near-atomic scale [34-36]. Comparatively, the APT result of the  $\gamma$ -austenite in the aged steel (Fig. 3(a)) shows that the reconstructed intragranular  $\kappa$ -carbides are distributed along a certain direction. The concentration profile in Fig. 3(b) shows the clear fluctuation of the different elements traversing the  $\gamma$ -austenite and  $\kappa$ -carbides. The  $\kappa$ -carbides are obviously rich in C and Al and poor in Fe, while the distributions of Mn and Cr between the  $\gamma$ -austenite and  $\kappa$ -carbide are almost uniform. Thus, putting together the HRSTEM and APT results clearly indicates that the chemical partitioning of solute

elements is unnecessary for the formation of the ordered  $\kappa$ -carbides.

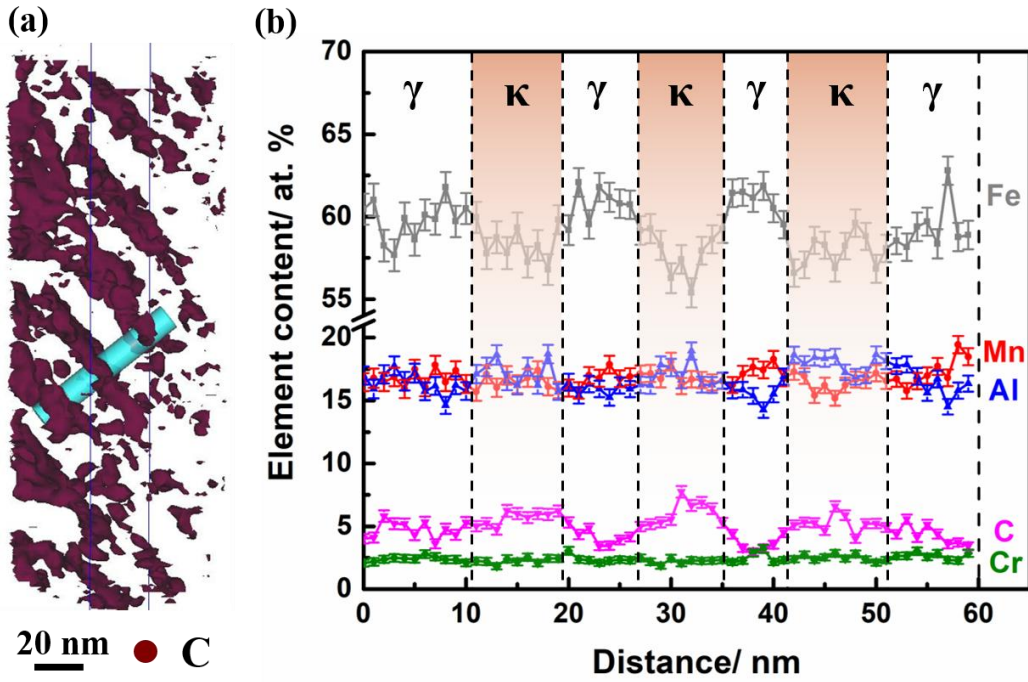


Fig. 3 APT characterization of  $\gamma$ -austenite in the aged steel: (a) reconstructed C map showing intragranular  $\kappa$ -carbides with an iso-concentration surface at 6 at. % C; (b) 1D concentration profile generated by the 10 nm diameter virtual cylinder in (a).

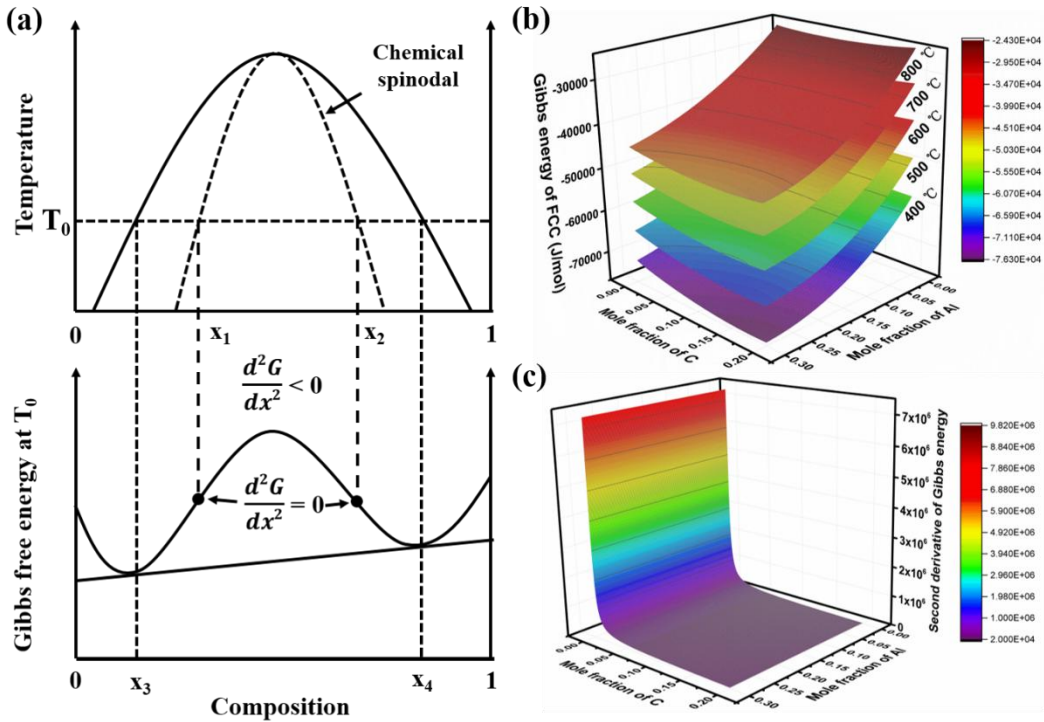


Fig. 4 (a) Schematic phase diagram of miscibility gap and the corresponding free energy curve [37]; (b) calculated Gibbs energy of FCC phase as a function of mole fractions of Al and C in

Fe-20Mn-9Al-3Cr-1.2C (wt. %) steel at the temperature range 400-800 °C; (c) calculated second derivative (curvature) of the Gibbs energy at 600 °C in (b).

Thermodynamically, the spinodal decomposition is a transformation without activation energy barrier and can result in a decreased total Gibbs energy [37]. When it occurs to the high temperature  $\gamma$ -austenite, the  $\gamma'$  and  $\gamma''$  phases form with the change of C and Al contents. Due to the same FCC crystal structure of the  $\gamma'$  and  $\gamma''$  phases, the Gibbs energy of both phases will move along the same Gibbs energy-composition curve. To ensure the decreased total Gibbs energy of FCC phase, the Gibbs energy-composition curve has a negative curvature [37], i.e.  $\frac{d^2G}{dx^2} < 0$ , as the same as the composition range between  $x_1$  and  $x_2$  shown in Fig. 4 (a). A small composition fluctuation decreases its total free energy to give rise to the spinodal decomposition by up-hill diffusion. Outside this composition range, a small composition fluctuation results in an increase of the free energy, which makes the alloy unstable. To decrease the total free energy, an energy barrier must be overcome so that the nucleation and growth mechanism dominates. The calculated results (Fig. 4(b)) show that the evolution trend of Gibbs energy of the FCC phase is the same at the large temperature range 400-800 °C. At each given temperature, the Gibbs energy decreases with increasing the mole fractions of Al and C, while its curvature remains always positive (the case of 600 °C shown in Fig. 4(c) and those of the other temperatures in [Supplementary](#)) ruling out the spinodal decomposition of  $\gamma \rightarrow \gamma' + \gamma''$ . It should be further noted that the calculated Gibbs energy in Fig. 4 (b) originates totally from the disordered FCC phase. The fact that the ordering reaction of  $\gamma'' \rightarrow L1_2$  phase has no contribution indicates that it is thermodynamically unfavorable.

According to the classical nucleation theory in solids [37], the minimum activation energy barrier for the  $\kappa$ -carbide precipitation in  $\gamma$ -austenite matrix is described as:

$$\Delta G^* = \frac{16\pi\gamma_{\kappa/\gamma}^3}{3(\Delta G_V - \Delta G_S)^2} \quad (1)$$

where  $\gamma_{\kappa/\gamma}$  is interfacial energy between the  $\kappa$ -carbides and  $\gamma$ -austenite,  $\Delta G_V$  is chemical driving force of  $\kappa$ -carbides per unit volume and  $\Delta G_S$  is elastic strain energy. In equation (1), the interfacial energy and elastic strain energy can be further expressed as [38]:

$$\gamma_{\kappa/\gamma} = \frac{\varepsilon(c-c_0)^2}{d^2} \quad (2)$$

$$\Delta G_S = \frac{E\delta^2(c-c_0)^2}{1-\nu} \quad (3)$$



$$\text{with lattice misfit } \delta = \frac{a_{\gamma} - a_{\kappa}}{a_{\kappa}} \quad (4)$$

where  $\varepsilon$  is pair interaction energy,  $c$  is nucleus composition,  $c_0$  is nominal composition,  $d$  is interface thickness,  $E$  is Young modulus,  $\nu$  is Poisson coefficient,  $a_{\kappa}$  and  $a_{\gamma}$  are lattice parameters of the  $\kappa$ -carbides and  $\gamma$ -austenite, respectively.

At the initial stage of the  $\kappa$ -carbide formation, the fully coherent interface between the  $\kappa$ -carbide and  $\gamma$ -austenite matrix is revealed in Fig. 1 (b). The interfacial energy of  $\kappa$ -carbide precipitates in Fe-Mn-Al-C steel was calculated to be 0.025 J/m<sup>2</sup> [29]. For comparison, it is much lower than the interfacial energy of 0.115 J/m<sup>2</sup> necessary to form GP zones from the Al matrix in Al-Cu alloy [39]. The lattice misfit ( $\delta$ ) between the  $\kappa$ -carbide and  $\gamma$ -austenite is estimated to about 0.27 % in term of the HRSTEM-HAADF image in Fig. 1 (c), which results in the low  $\Delta G_S$  (measured lattice parameters in Supplementary). More importantly, the nearly consistent composition between the  $\kappa$ -carbides and  $\gamma$ -austenite matrix revealed by APT (see Fig. 2) indicates that the critical nucleation composition of  $\kappa$ -carbide can be very close to that of the  $\gamma$ -austenite matrix, which makes the value of  $(c - c_0)$  close to zero. All the results mean that there are both very low interfacial energy and elastic strain energy at the initial stage of  $\kappa$ -carbide formation. Therefore, the activation energy barrier to the nucleation of  $\kappa$ -carbides in  $\gamma$ -austenite matrix should be rather small. In addition, the large undercooling, due to a high cooling rate of more than 10<sup>3</sup> K/s during the near-rapid solidification [21], also increases the driving force for  $\kappa$ -carbide precipitation [37, 40].

Table 1 Quantitative chemical compositions of  $\gamma$ -austenite matrix and  $\kappa$ -carbide precipitates in the as-cast and aged steels obtained by APT analyses (in at. %).

| Steel   | Phase           | Fe           | Mn           | Al           | C           | Cr          |
|---------|-----------------|--------------|--------------|--------------|-------------|-------------|
| As-cast | $\gamma/\kappa$ | 58.42 ± 0.45 | 16.73 ± 0.11 | 17.50 ± 0.25 | 4.87 ± 0.25 | 2.48 ± 0.11 |
|         | $\gamma$        | 60.41 ± 0.50 | 16.71 ± 0.13 | 15.95 ± 0.27 | 4.39 ± 0.26 | 2.54 ± 0.07 |
| Aged    | $\kappa$        | 56.00 ± 0.29 | 16.43 ± 0.12 | 18.22 ± 0.22 | 6.37 ± 0.25 | 2.45 ± 0.17 |

Further, density functional theory calculations [41, 42] suggest that the Fe, Mn and Cr atoms are usually considered to be located at the face center positions of the ideal (Fe, Mn)<sub>3</sub>AlC lattice. Assuming that such positions in the initially formed  $\kappa$ -carbide are completely occupied and as shown in Table 1, the occupancy rates of Al and C atom positions are determined to be 67.6 % and 18.8 %, respectively. This indicates that there is a large amount of quenched-in vacancies in the  $\kappa$ -carbides effectively promoting nucleation by increasing diffusion rates or relieving misfit strain energies [37]. Simultaneously, the presence of vacancies is a critical way to achieve ordering structures in non-stoichiometric phases [37]. The formation of an

ordered structure by nucleation only requires the short-range movement of atoms in a crystal lattice, which is much easier to achieve than the spinodal decomposition [43].

With the growth of  $\kappa$ -carbides after the aging treatment, their composition gradually approaches the equilibrium composition with the higher contents of Al and C. The interfacial energy and elastic strain energy also increase by the increased composition difference ( $c - c_0$ ) between the  $\kappa$ -carbides and  $\gamma$ -austenite matrix (see Table 1), and the increased lattice misfit ( $\delta$ ) of 2.27 % obtained by HRSTEM-HAADF image (Fig. 1 (f)) and equation (4). The increased lattice misfit ( $\delta$ ) resulted from the partitioning of Al and C to the  $\kappa$ -carbides [4, 7, 12]. This indicates that nucleation of the equilibrium  $\kappa$ -carbides directly in the  $\gamma$ -austenite matrix is difficult. Therefore, there must be a change in composition and associated crystal structure accompanying with the nucleation and growth process.

In summary, the formation mechanism of the intragranular  $\kappa$ -carbide in  $\gamma$ -austenite of the austenite-based Fe-20Mn-9Al-3Cr-1.2C low-density steel was revisited in terms of (HR)STEM, APT and thermodynamic calculation. It was experimentally observed that the  $\kappa$ -carbide precipitates of 2-3 nm in particle size were homogeneously distributed in  $\gamma$ -austenite of the as-cast steel. They corresponded to the ordered  $L'1_2$  structure without elemental partitioning at near-atomic scale. The thermodynamic calculations indicated that the Gibbs energy of the FCC phase always had a positive curvature with the variable contents of Al and C in the temperature range 400-800 °C. These results clearly show that the formation of the intragranular  $\kappa$ -carbide in the as-cast and aged steels obeys the nucleation and growth mechanism rather than the well-known spinodal decomposition-ordering mechanism. The similar lattice structure, same composition and complete coherency between the  $\gamma$ -austenite and  $\kappa$ -carbide resulted in an extremely low nucleation barrier. With the growth of  $\kappa$ -carbides after aging, their composition tended to be stable, which increased the composition fluctuation between the  $\gamma$ -austenite and  $\kappa$ -carbide.

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