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The importance of simulation the four core effects of Multi-principal element alloys based on the inherent sublattice preference of atoms

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INTRODUCTION & AIM

1. Special quasirandom structure (SQS) based on the prefect random mixing hypothesis is insufficient to simulate the four core effects of Multi-principal element alloys (MPEAs) or high/ medium entropy alloys (HEAs/MEAs), as the SQS model ignores ① the difference between the constituent atoms, ② the difference between the different crystal lattice structure, such as FCC, BCC and HCP, and ③ the effect of the different heat treatment temperatures.
2. We realize that the inherent sublattice preference of atoms should be and could be considered at current stage, or else, the simulation of HEAs is not reliable based on SQS.
3. We supply a set of reasonable and comprehensive solutions based on sublattice model to quantitatively and graphically characterize the four core effects

METHOD

1. Structure model assessment.

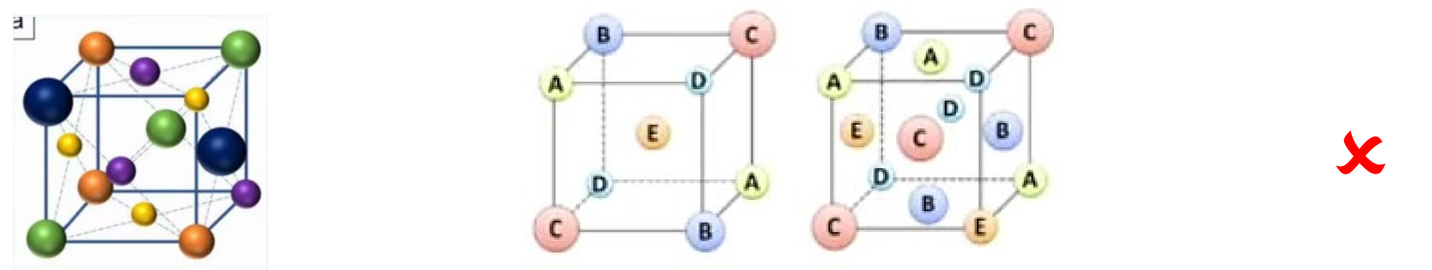


Fig.1 It is insufficient to describe HEAs using unit cell, which are modelled commonly.

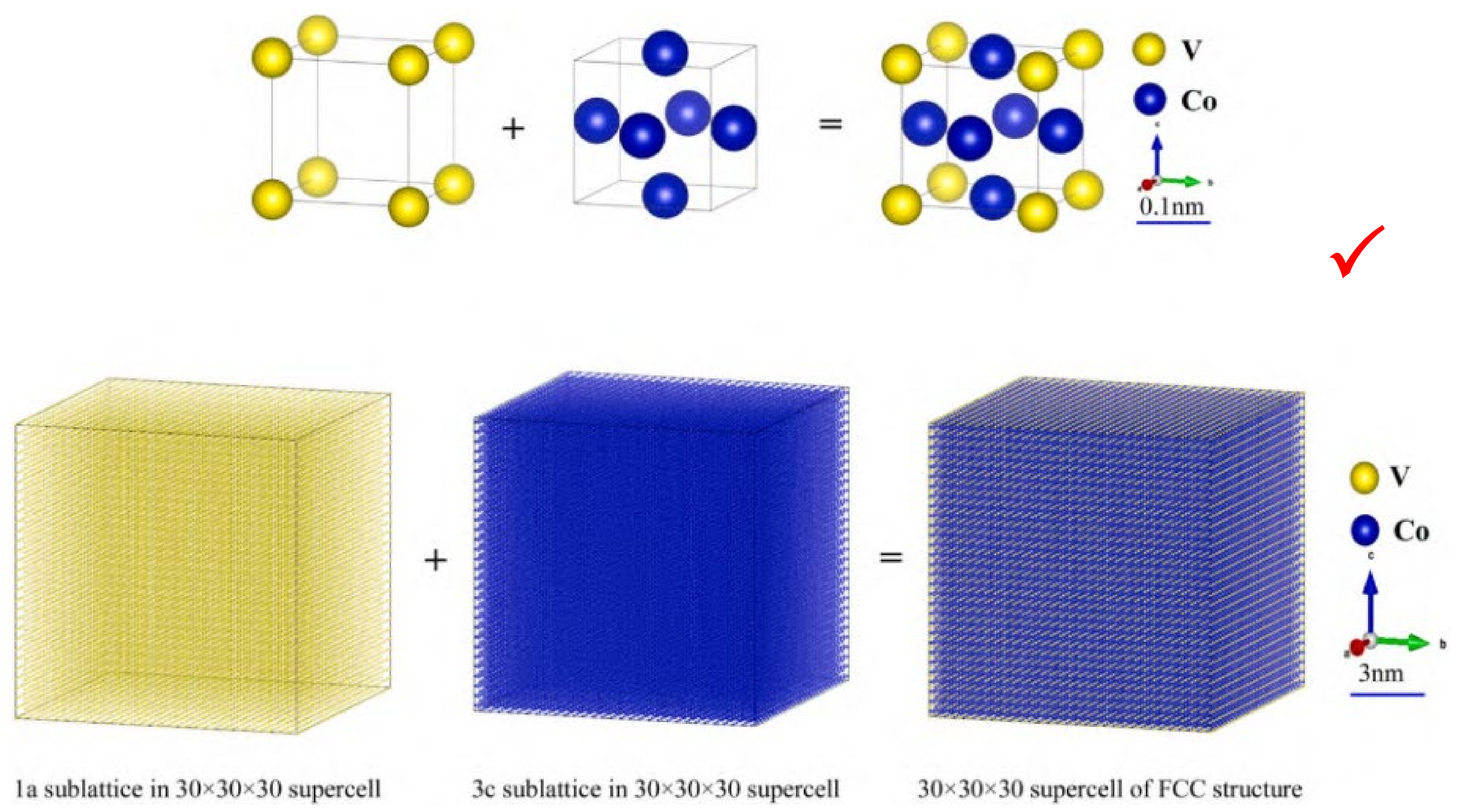
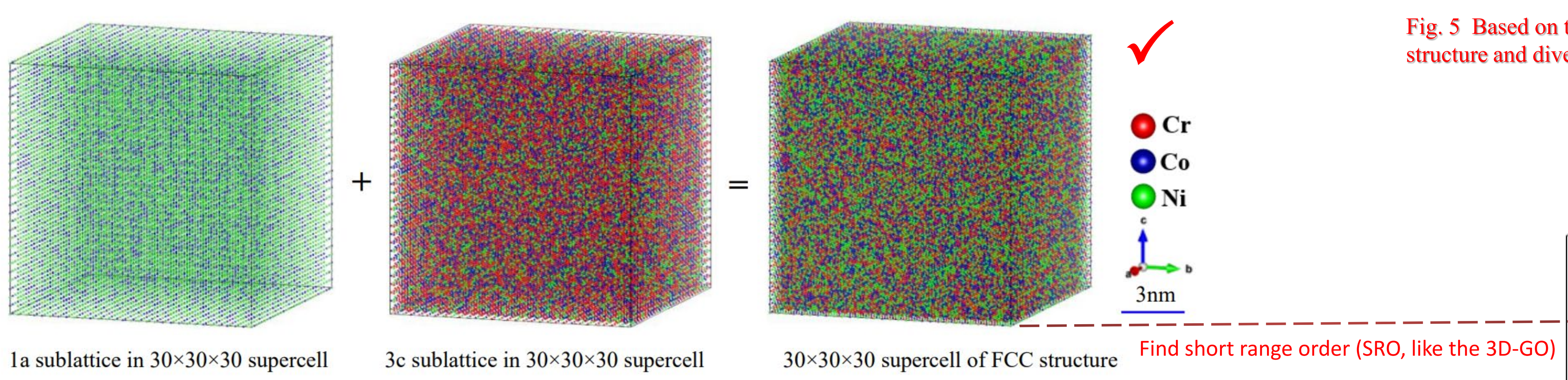


Fig. 4. The unit cell and supercell of the ordered $L1_2$ prototype structure



$(Co_{0.3581}Cr_{0.0005}Ni_{0.6414})_{1a}+(Co_{0.3251}Cr_{0.4442}Ni_{0.2307})_{3c}=(Co_{0.3581}Cr_{0.0005}Ni_{0.6414})_{1a}(Co_{0.3251}Cr_{0.4442}Ni_{0.2307})_{3c}$

$Co_{9490}Cr_{13}Ni_{17497} + Co_{26510}Cr_{35987}Ni_{18503} = Co_{36000}Cr_{36000}Ni_{36000}$

Fig.2 The reasonable approach to describe HEAs using supercell based on the predicted sublattice occupying fractions (SOFs)

2. Predicting the SOFs ($y_{M_i}^{S_j}$) using sublattice model. Here FCC_$L1_2$ models were shown.

$$33.33Co+33.33Cr+33.34Ni=25[y_{Co}^{1a}(Co)+y_{Cr}^{1a}(Cr)+y_{Ni}^{1a}(Ni)]+75[y_{Co}^{3c}(Co)+y_{Cr}^{3c}(Cr)+y_{Ni}^{3c}(Ni)]$$

Construct the thermodynamic function equation of Gibbs free energy of formation, ΔG_f

$$Co,Cr,Fe,Ni \xrightarrow{①} (Co_{y_{Co}^{1a}},Cr_{y_{Cr}^{1a}},Fe_{y_{Fe}^{1a}},Ni_{y_{Ni}^{1a}})_{1a}(Co_{y_{Co}^{3c}},Cr_{y_{Cr}^{3c}},Fe_{y_{Fe}^{3c}},Ni_{y_{Ni}^{3c}})_{3c}$$

② ③

$(Co)_{1a}(Co)_{3c}$	$(Co)_{1a}(Cr)_{3c}$	$(Co)_{1a}(Fe)_{3c}$	$(Co)_{1a}(Ni)_{3c}$
$(Cr)_{1a}(Co)_{3c}$	$(Cr)_{1a}(Cr)_{3c}$	$(Cr)_{1a}(Fe)_{3c}$	$(Cr)_{1a}(Ni)_{3c}$
$(Fe)_{1a}(Co)_{3c}$	$(Fe)_{1a}(Cr)_{3c}$	$(Fe)_{1a}(Fe)_{3c}$	$(Fe)_{1a}(Ni)_{3c}$
$(Ni)_{1a}(Co)_{3c}$	$(Ni)_{1a}(Cr)_{3c}$	$(Ni)_{1a}(Fe)_{3c}$	$(Ni)_{1a}(Ni)_{3c}$

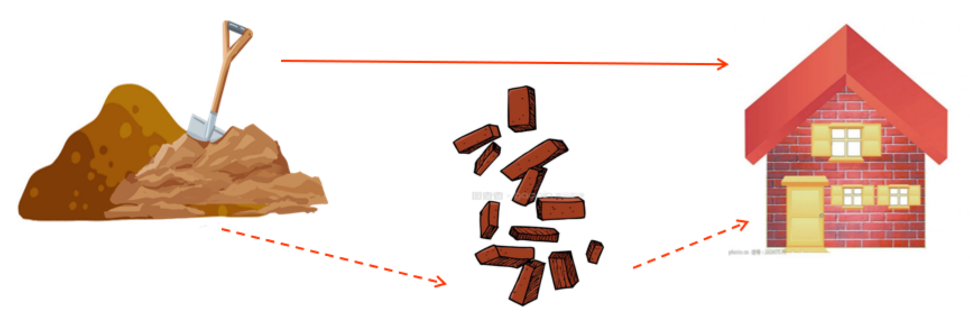


Fig. 3 The alternative computation path of the thermodynamic function, i.e., ΔG①=ΔG②+ΔG③.

$$\Delta G=\sum_{i=1,2,\dots n}\sum_{j=1,2,\dots n} y_{M_i}^{1a}y_{M_j}^{3c}\Delta G_{(M_i^{1a}:M_j^{3c})}-T\cdot(-R\left(0.25\times\sum_{i=1}^{n}y_{M_i}^{1a}\times ln y_{M_i}^{1a}+0.75\times\sum_{i=1}^{n}y_{M_i}^{3c}\times ln y_{M_i}^{3c}\right)$$

RESULTS & DISCUSSION

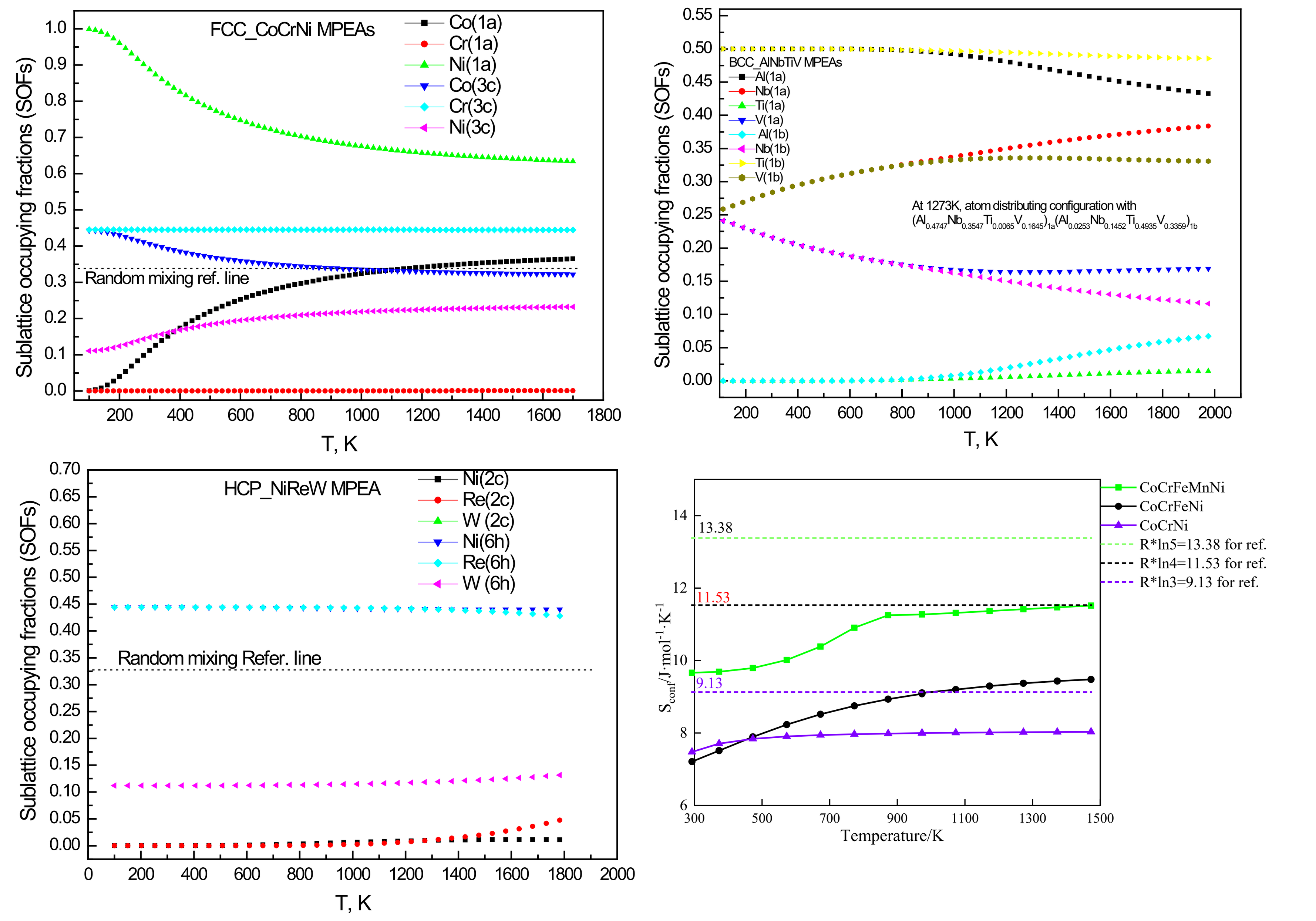
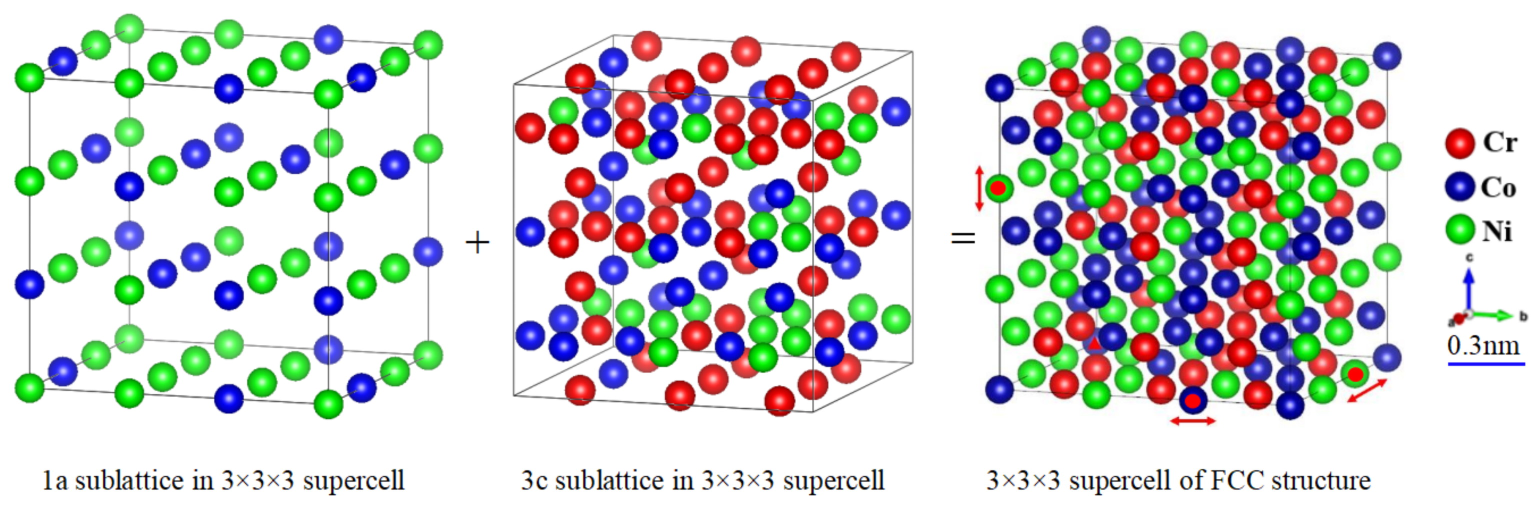


Fig. 4 The temperature- and composition-dependent sublattice occupying fractions of different MPEAs and thus the configurational entropy based on SOFs and SQS models. The inherent sublattice preference should be and could be considered.

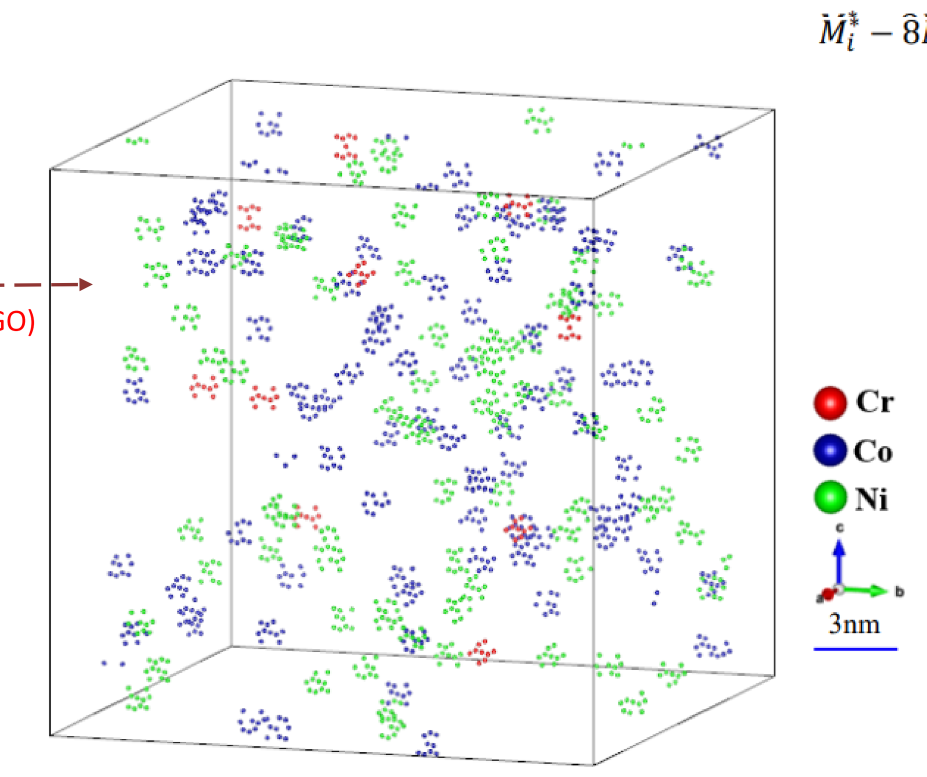


$(Co_{0.3581}Cr_{0.0005}Ni_{0.6414})_{1a}+(Co_{0.3251}Cr_{0.4442}Ni_{0.2307})_{3c}=(Co_{0.3581}Cr_{0.0005}Ni_{0.6414})_{1a}(Co_{0.3251}Cr_{0.4442}Ni_{0.2307})_{3c}$

$Co_{10}Ni_{17} + Co_{26}Cr_{36}Ni_{19} = Co_{36}Cr_{36}Ni_{36}$

Fig. 5 Based on the predicted SOFs and computing power, we establish the atom distributing model to calc. the fine lattice structure and diverse properties. i.e., the four core-effects of MPEAs, more detail see our published papers in Reference list

$M_i^*-8M_i$



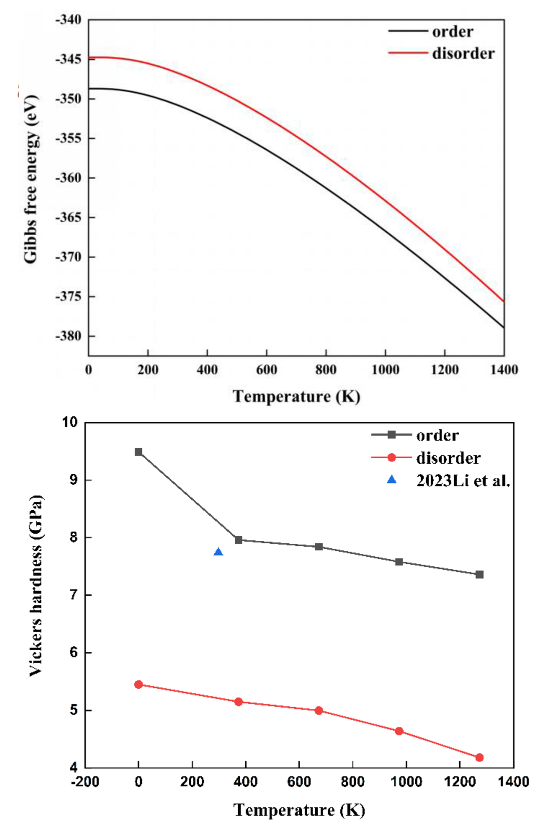


Fig. 6 The $M_i^*-8M_i$ and above (containing $M_i^*-9M_i$ and $M_i^*-10M_i$) coordinating clusters

Fig. 7 Thermodynamic and physical properties of FCC_CoNiV MPEAs

CONCLUSION

1. It is important to quantitatively and graphically characterize the four core effects, based on the inherent sublattice preference of atoms, which extends beyond the commonly believed but baseless SQS based on the random mixing hypothesis. Or else it will miscalculate the crystal lattice structure and diverse properties of MPEAs.
2. Frankly speaking, in our view, We are the first-time, and the only group to realize and establish series models and solutions to quantitatively and graphically characterize the four core effects based on the inherent sublattice preference of atoms.
3. Based on these reasonable and general structural model and approaches, high-through calculations and experimental verified work is set up to enrich the database of MPEAs and thus AI for MPEAs.

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