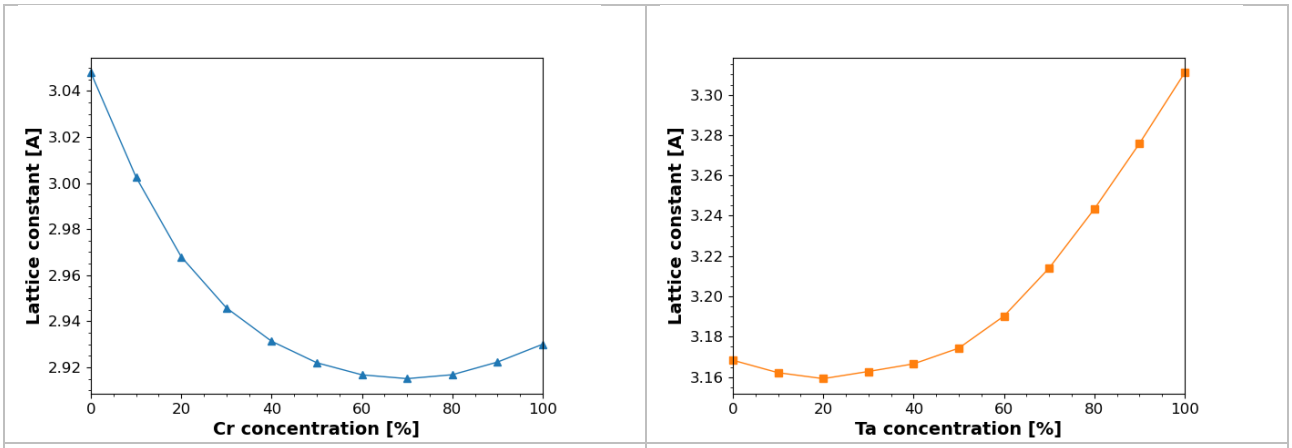
Additional data

Here some additional data regarding the molecular dynamics models and results re provided. Although the information in the main manuscript are believed to be self-sustaining, these data may help the most curious readers.

1. Quasi-static model

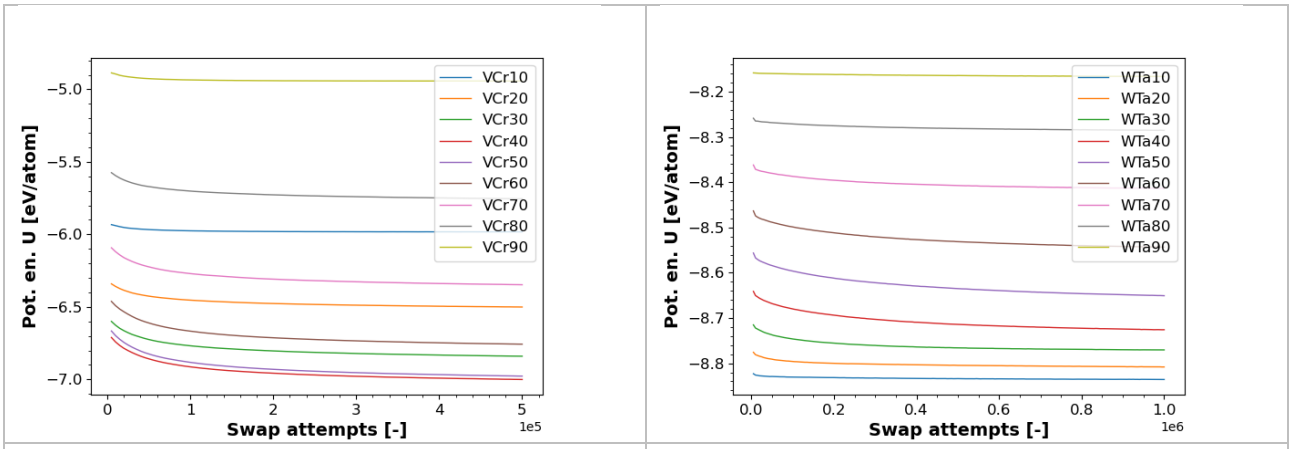
Additional data computed in the quasi-static model. Figure 1 shows the system lattice constant of VCr and WTa systems.



(a) (b)

Figure 1 – Lattice constant vs concentration for VCr_x (a) and WTa_x (b).

Figure 2 shows the annealing effect of the Monte Carlo + Molecular Dynamics (MC+MD) hybrid method. (a) and (b) show the reduction in potential energy. (c) and (d) show the acceptance rate of the swaps. It shows that the systems got close to the minimum potential energy possible, so to the most stable system possible.



(a) (b)

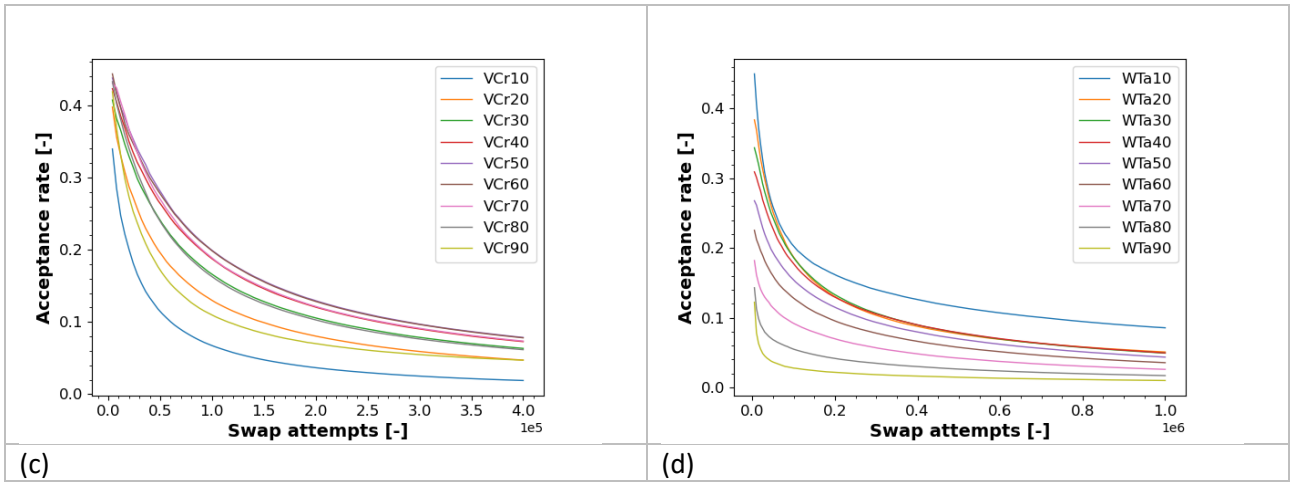


Figure 2 – Potential energy normalized on the system number of atoms (U) [eV/atom] vs swap attempts in the MC+MD method for VCr_x system (a) and WTa_x system (b). Acceptance rate of the swap in the MC+MD method for Vcr_x (c) and WTa_x (d).

2. Migration energy barrier model

Figure 3 shows the additional data regarding the Migration Energy Barriers (MEB) evaluations with the nudged elastic band method. The evolution of mean values and standard deviations with the sampled defect migrations is shown. It shows that the both the mean value and the standard deviation are stabilized. The standard deviations does not keep decreasing with increasing number of sample because of the heterogeneity of MEB values in mixed systems.

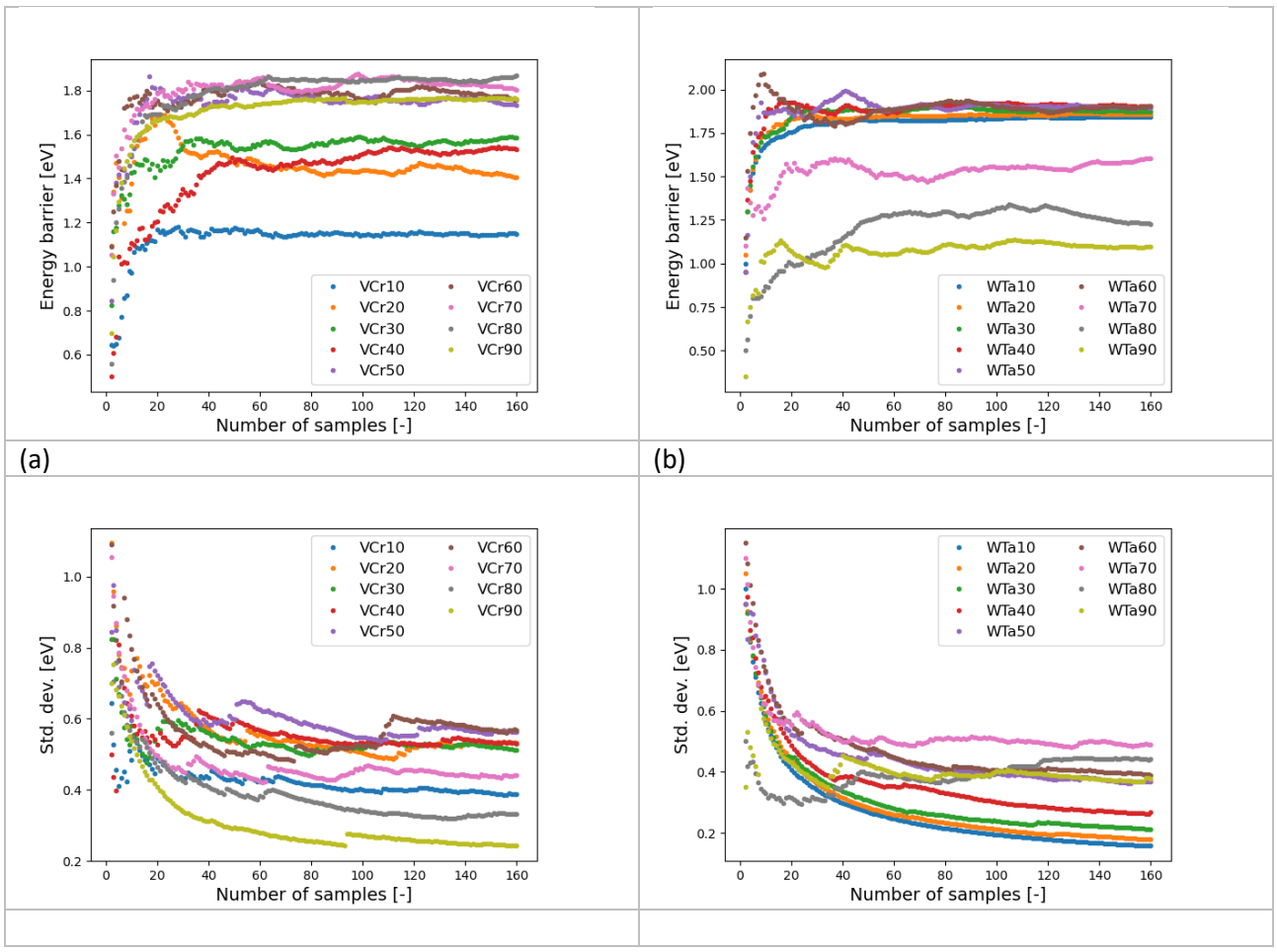


Figure 3 – Average migration energy barrier value vs the number of sampled defect migrations for VCr_x system (a) and WTa_x system (b). Average migration energy barrier value vs the number of sampled defect migrations for VCr_x system (c) and WTa_x system (d).

3. Damage model

Figure 4 and Figure 5 show the evolution of the system potential energy with the increase of collisional cascades. Figure 4 shows an example of the increase in average potential energy U [eV/atom] in the WTa_{80} system as an example. Figure 5 shows the relative potential energy evolution computed as follows:

$$U_{rel,i} = abs\left(\frac{U_0 - U_i}{U_0}\right)$$

Where $U_{rel,I}$ is the relative potential energy at i-th cascade, U_0 is the average potential energy before irradiation phase starts and U_i is the average potential energy of the system at the i-th cascade.

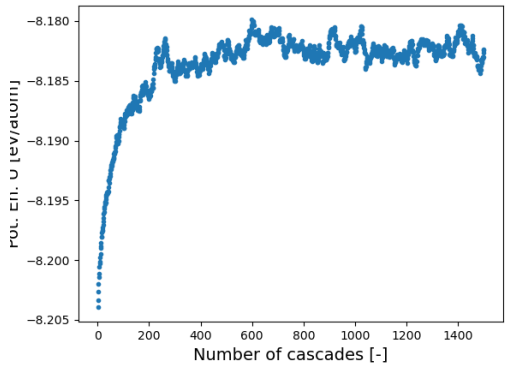


Figure 4 – Potential energy per atom U [eV/atom] vs number of cascades, WTa_{80} example.

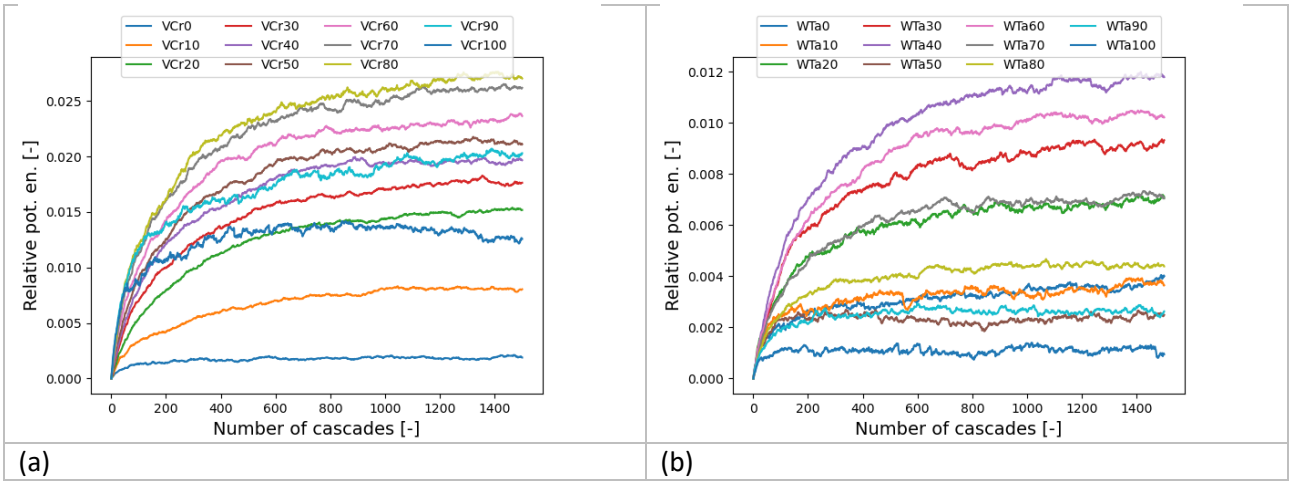
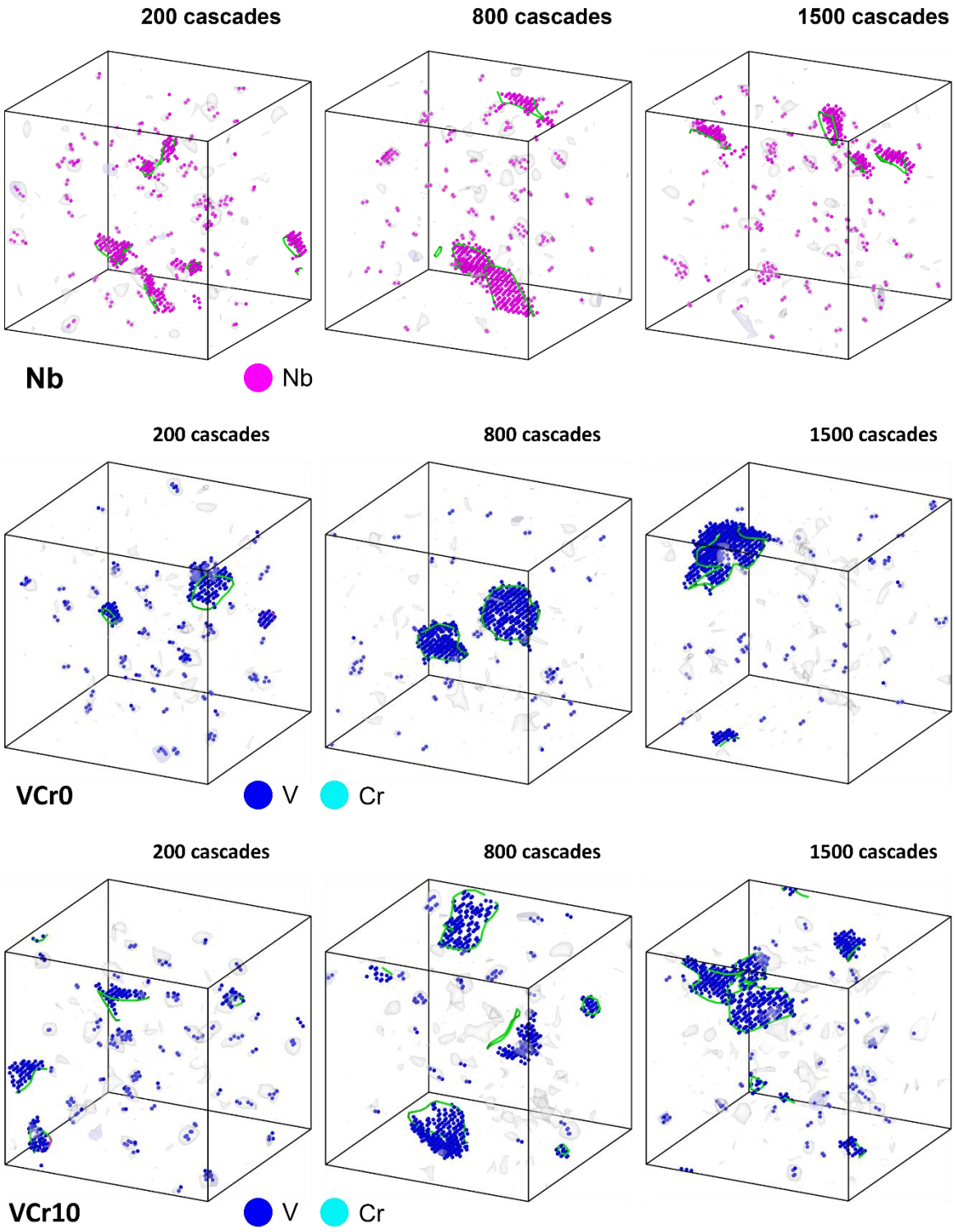
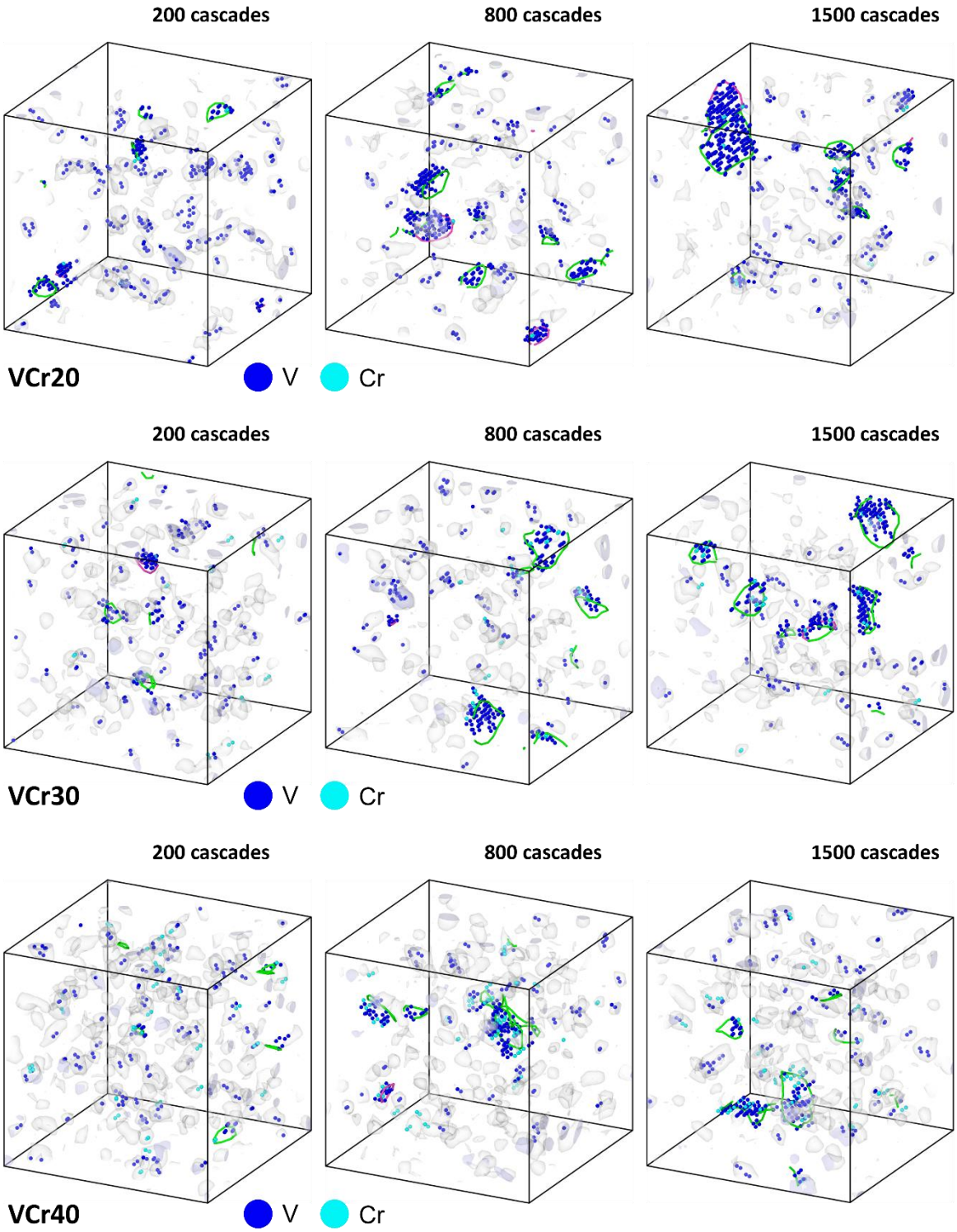
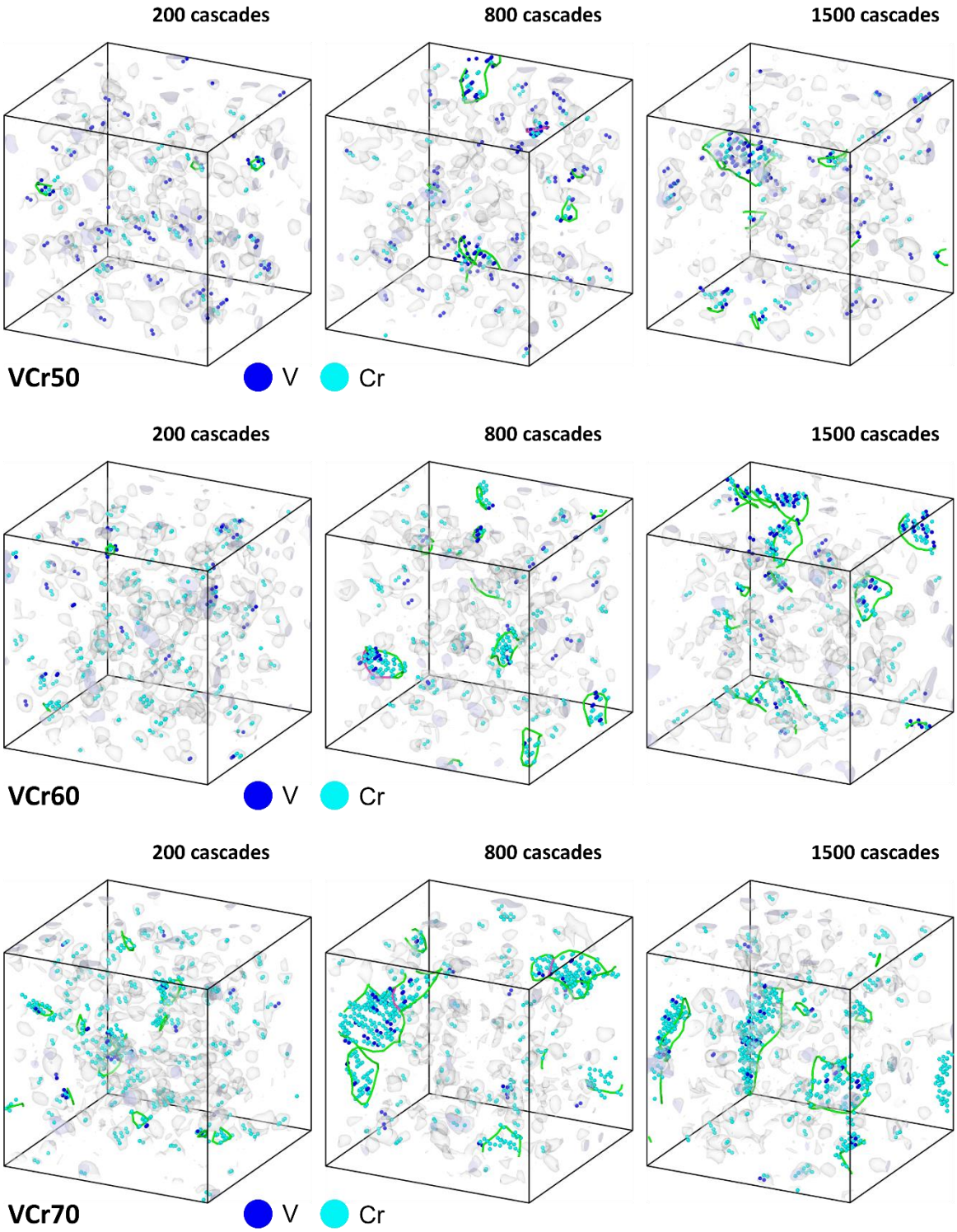


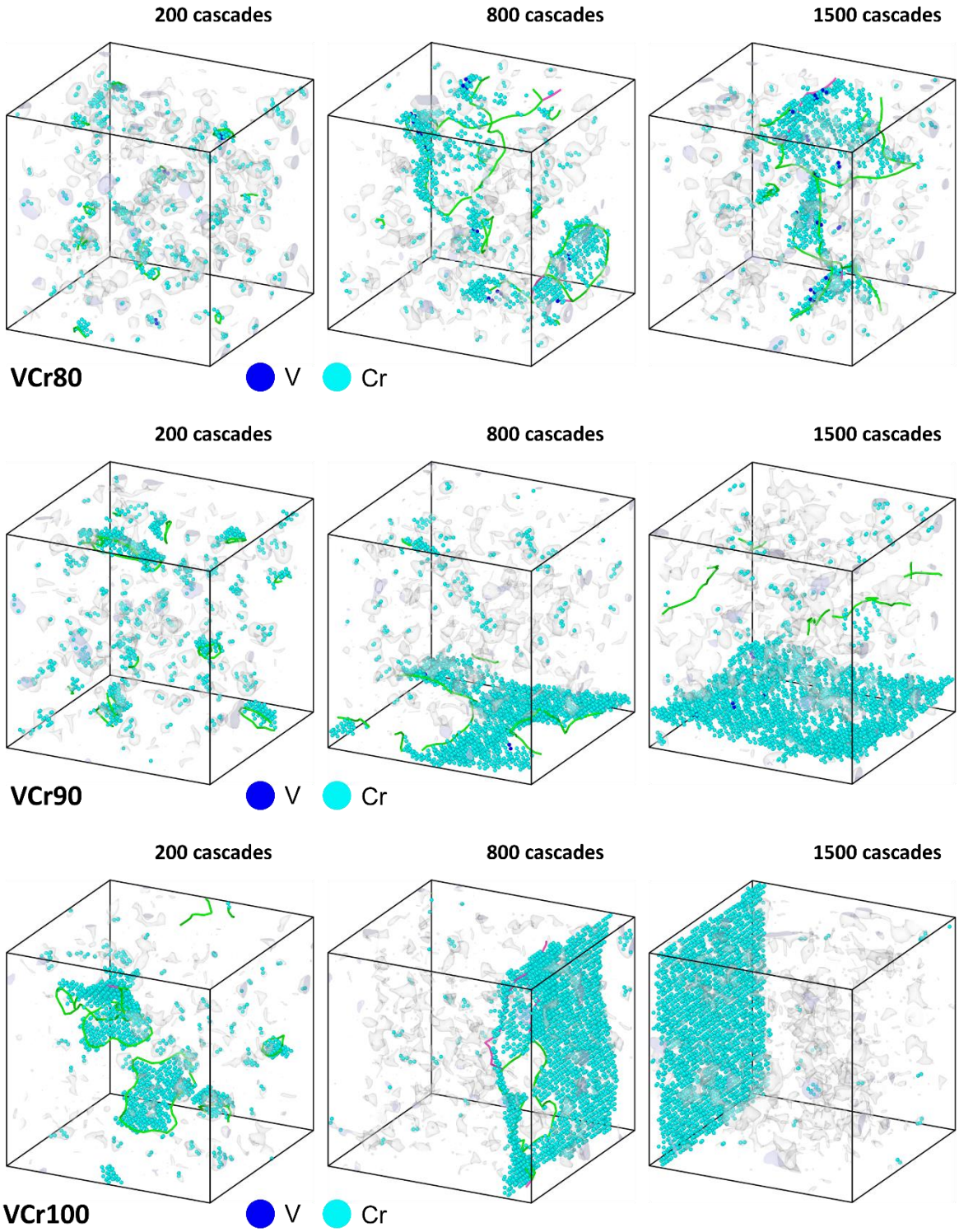
Figure 5 – Relative potential energy vs number of cascades for VCr_x system (a) and WTa_x system (b).

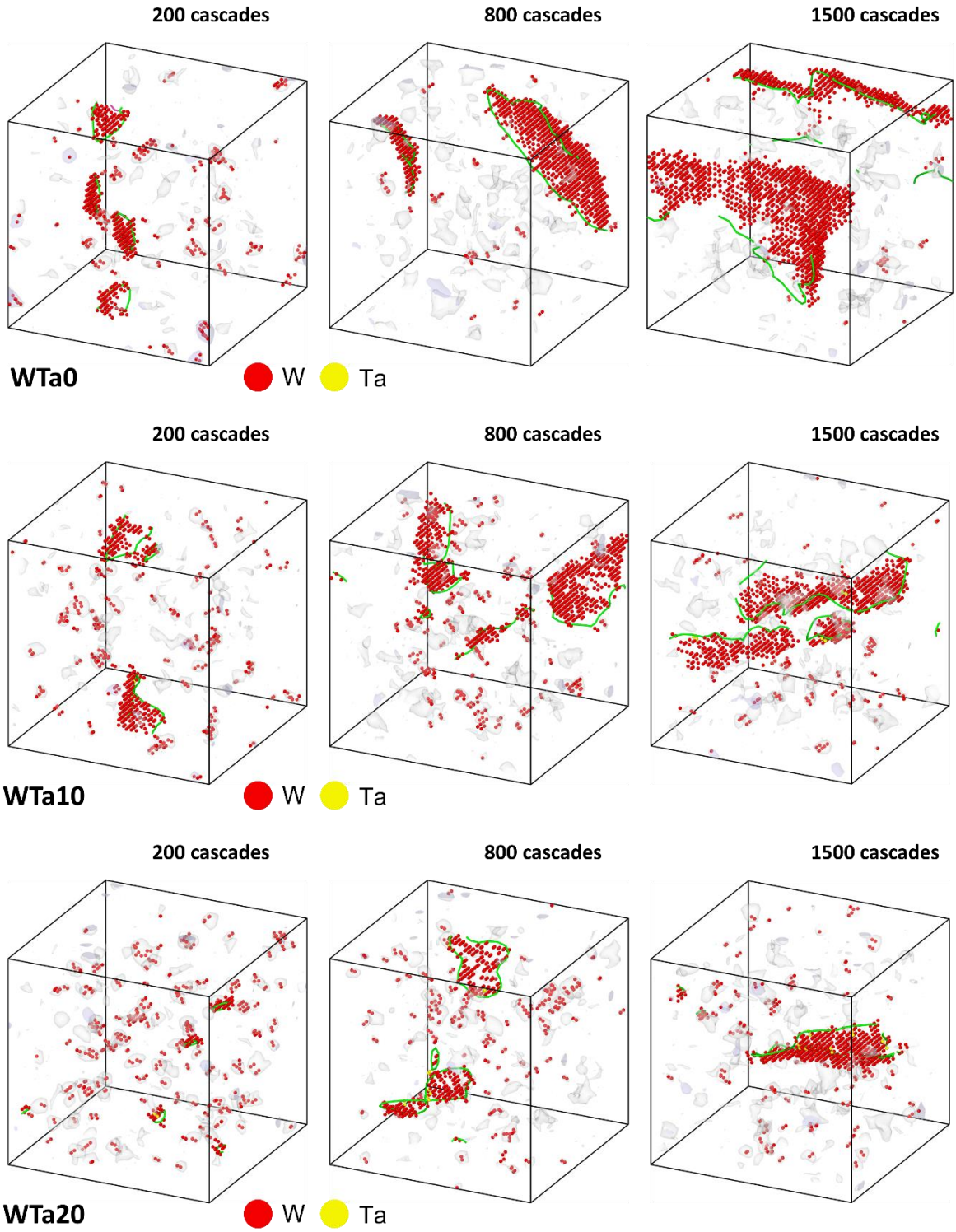
Below there are the pictures of the defects and defect clusters at 200, 800 and 1500 cascades for all the systems simulated in this work (Nb, VCr_x and WTa_x).

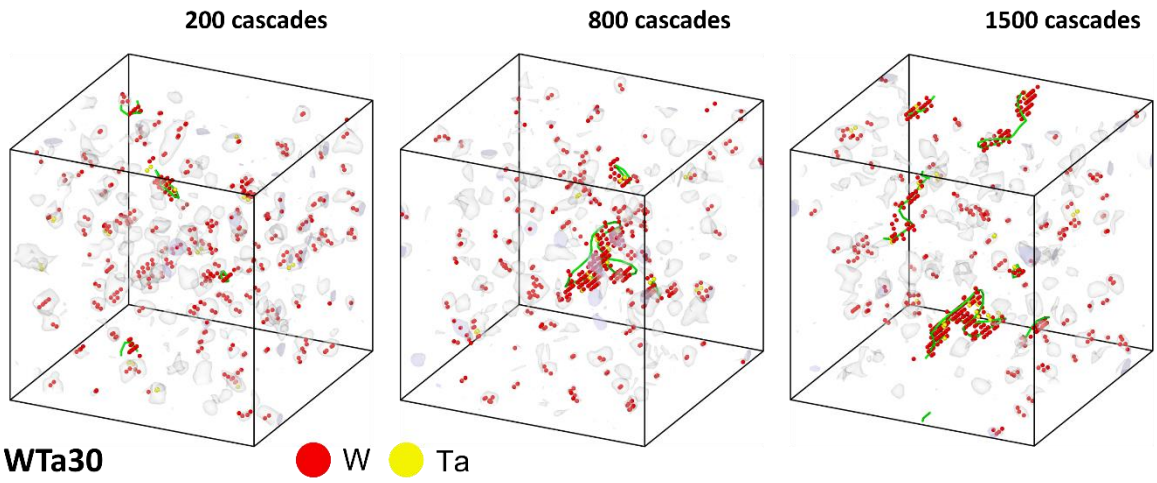

200 cascades
800 cascades
1500 cascades
Nb
Nb
200 cascades
800 cascades
1500 cascades
VCr0
V
Cr
200 cascades
800 cascades
1500 cascades
VCr10
V
Cr

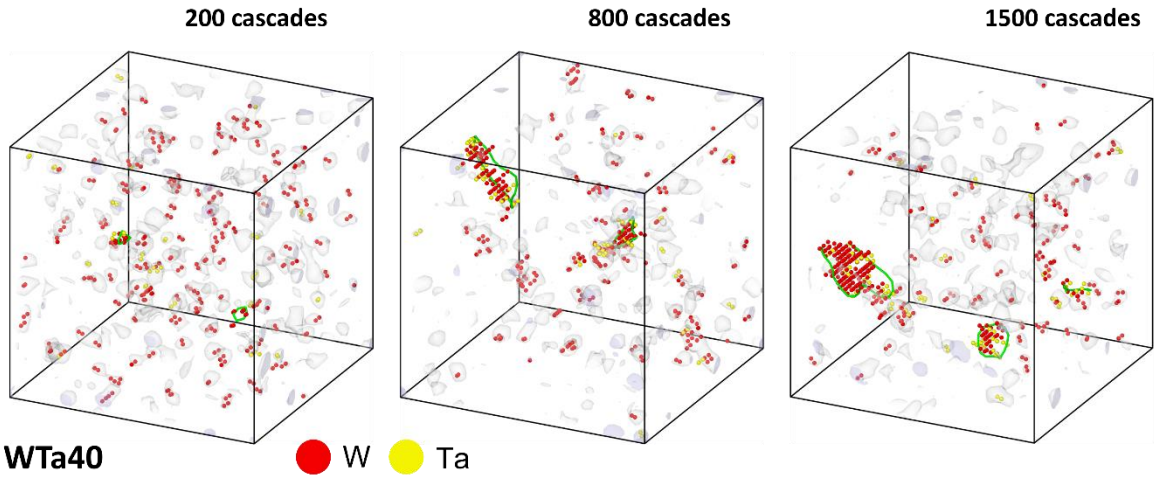

200 cascades
800 cascades
1500 cascades
VCr20
V
Cr
200 cascades
800 cascades
1500 cascades
VCr30
V
Cr
200 cascades
800 cascades
1500 cascades
VCr40
V
Cr

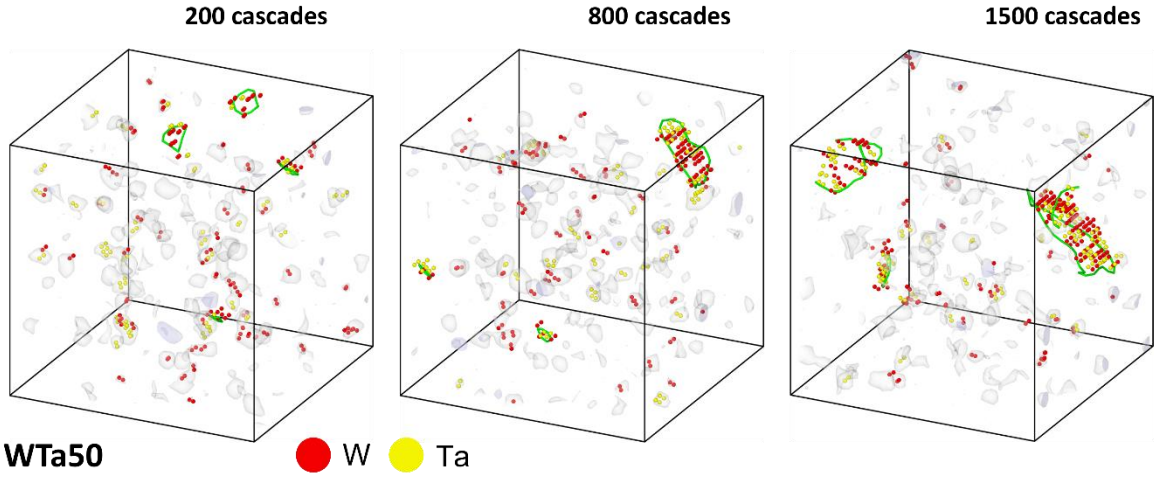

200 cascades
800 cascades
1500 cascades
VCr50
V
Cr
200 cascades
800 cascades
1500 cascades
VCr60
V
Cr
200 cascades
800 cascades
1500 cascades
VCr70
V
Cr

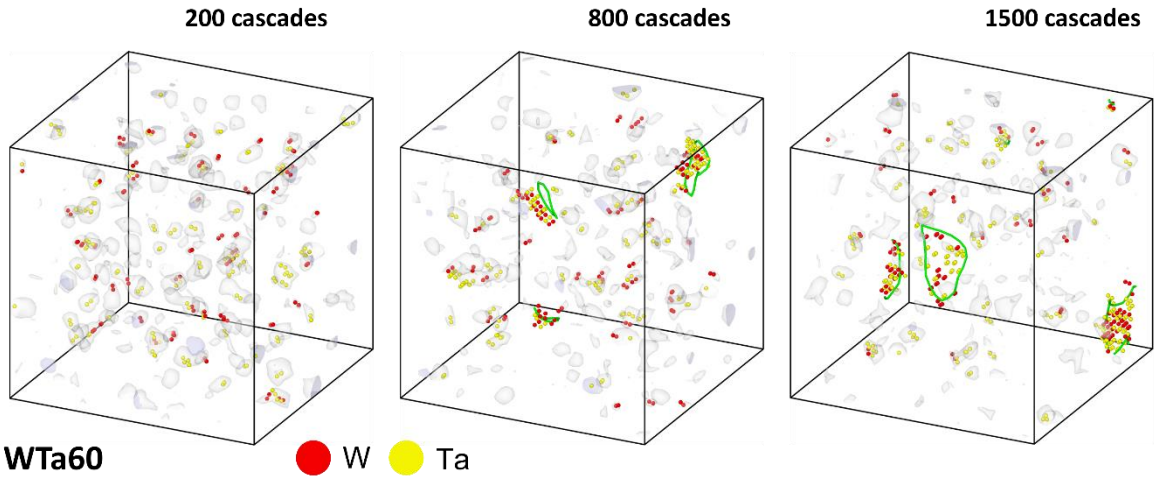

200 cascades
800 cascades
1500 cascades
VCr80
V
Cr
200 cascades
800 cascades
1500 cascades
VCr90
V
Cr
200 cascades
800 cascades
1500 cascades
VCr100
V
Cr

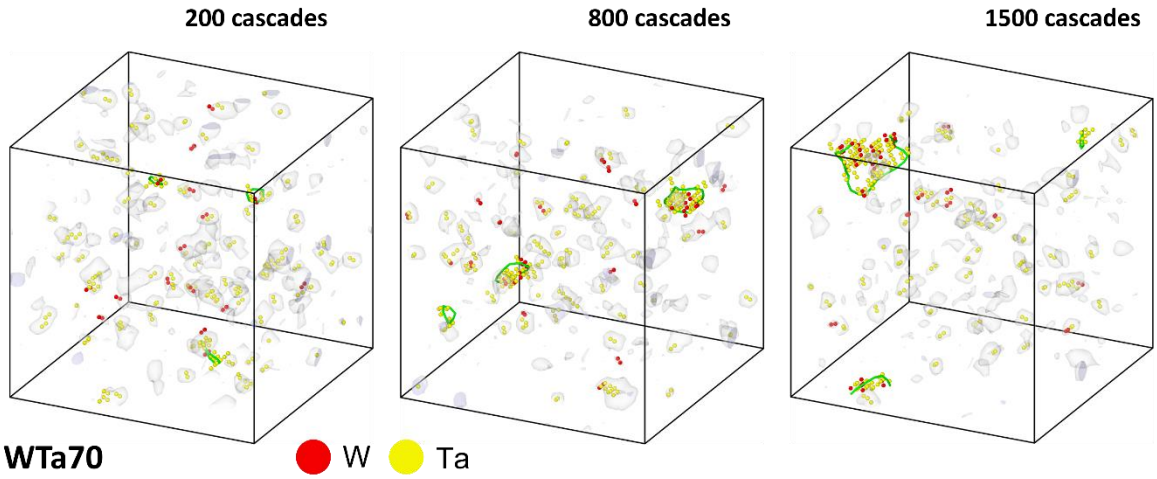

200 cascades
800 cascades
1500 cascades
WTa0
W
Ta
200 cascades
800 cascades
1500 cascades
WTa10
W
Ta
200 cascades
800 cascades
1500 cascades
WTa20
W
Ta

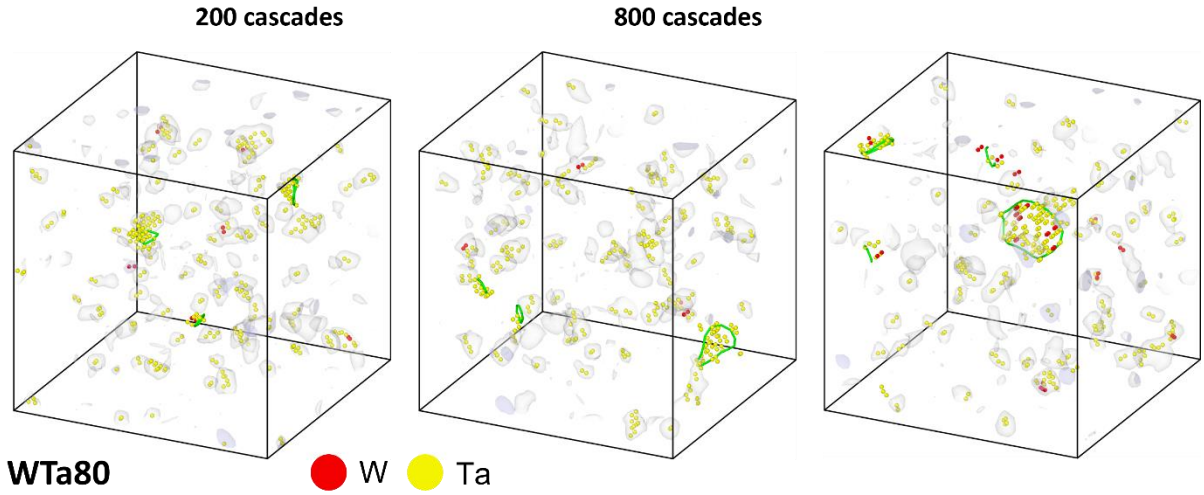

200 cascades
800 cascades
1500 cascades
WTa30
W
Ta

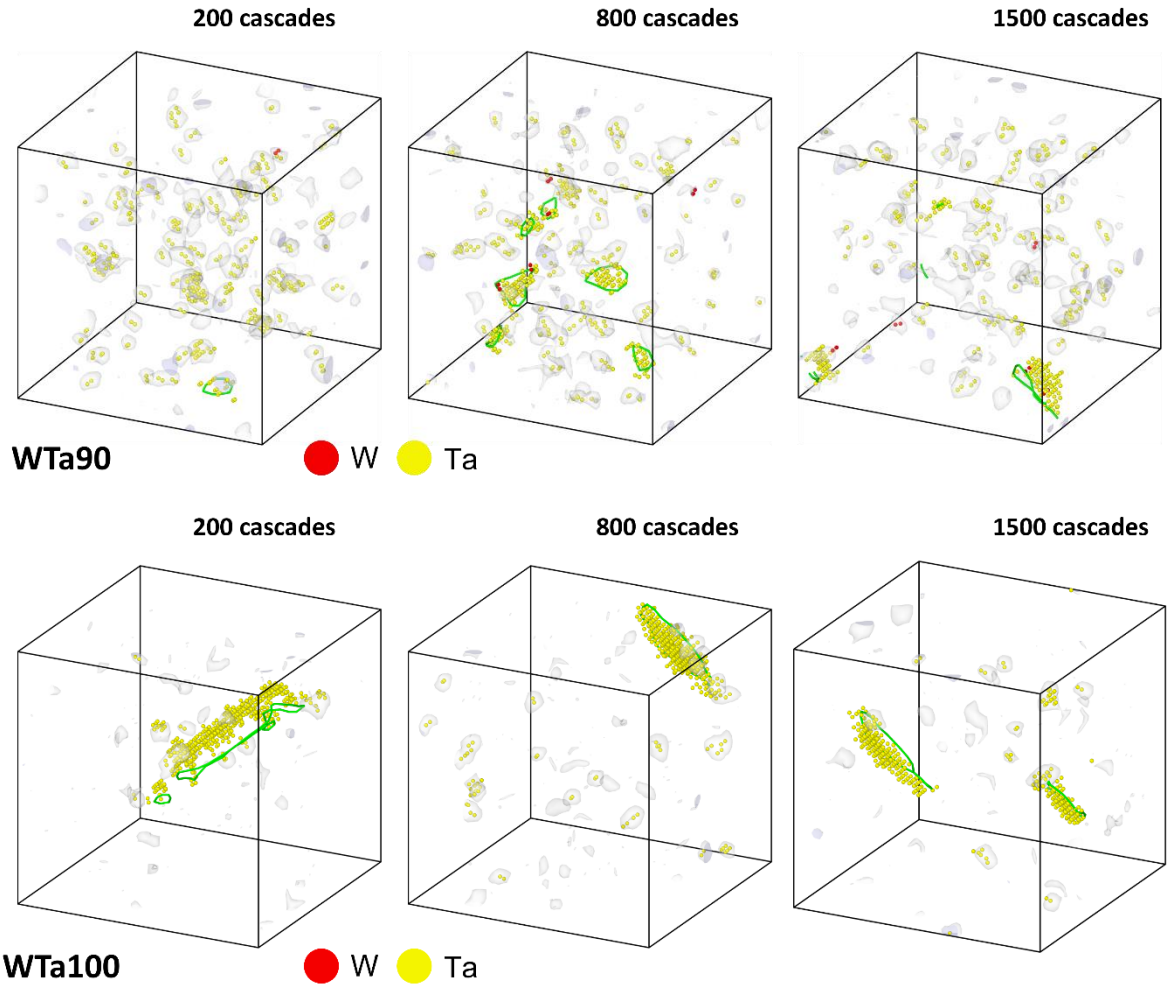

200 cascades
800 cascades
1500 cascades
WTa40
W
Ta


200 cascades
800 cascades
1500 cascades
WTa50
W
Ta


200 cascades
800 cascades
1500 cascades
WTa60
W
Ta


200 cascades
800 cascades
1500 cascades
WTa70
W
Ta


200 cascades
800 cascades
WTa80
W
Ta


200 cascades
800 cascades
1500 cascades
WTa90
W
Ta
200 cascades
800 cascades
1500 cascades
WTa100
W
Ta