# Reviewer 1:

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| No. | Comment | Response |
| 1 | Equation 1 is only applicable to zero K. At elevated temperature, equation 1 may be wrong for calculating interfacial energy because entropy term cannot be ignored (Temp \* entropy is not zero anymore!). Authors must address the entropy effect and how it changed the interfacial energy. Without the discussion regarding to entropy effect, all the results about the effect of temperature on energetic calculations are quite questionable. | Thank you for your comment. Here the ‘interfacial energy’ used in equation 1, is the internal energy (potential energy plus kinetic energy) not the free energy. Hence, entropy effect is out of the scope of the current work. |
| 2 | In Figure 4, why the GB anisotropy is considered as a function of GB type? This figure only shows the A\_type GB. The author should elaborate further on it. | In equation 3, it is noted that, ‘A\_type’ is the nomenclature for the GB anisotropy, not the ‘type A STGB’. We will change this confusing nomenclature. GB anisotropy is considered as a function of GB type to illustrate that GB energy in alpha U depends not only on misorientation angle but also in tilt plane and shear plane of GBs. We will add more elaborate discussion on this. |
| 3 | In page 11, author claimed that "Thu current work indicates that at lower temperature, there is less driving force for grain growth due to the lower grain boundary energy". Indeed, it is well known that the slow grain growth at low temperature can be also ascribed to slow diffusion of grain boundary. Hence, it is not persuasive to demonstrate that the slow grain growth is due to low GB energy. | We agree with reasoning of slow grain growth by slow diffusion of grain boundary. But grain boundary migration is a function of driving force, and curvature driving force is one of them which is proportional to the GB energy. So, at lower temperature due to low GB energy, there will be less driving force for grain growth. From this perspective, we have claimed this statement. |
| 4 | In page 11, author mentioned stable fine-grained microstructure may hinder dislocation movement and lead to lower ductility. I suggest author to perform tensile study for some representative GBs (e.g., low GB energy vs. high GB energy) and analyze how these GBs response with external loadings at different temperatures. Otherwise, it is hard to understand the GB with low energy can lower ductility at lower temperature. | Thank you for your thoughtful insight. As per existing literature, there must be some correlation between GB energy and elastic modulus of the bi-crystal system. The reason behind the current statement is, as low GB energy of STGB leads to a finer microstructure and a finer microstructure has a lots of GBs (acts as stress concentrators) which leads to lower ductility. Our goal is not to determine the elastic property of different bi-crystal system along with their temperature dependence. |
| 5 | The legends labelled in some figures are too similar, e.g., Figure 5, which is hard to discern difference between them. I suggest using different line styles, colors, and maker styles to optimize all figures. | Thank you for your suggestion. We will update the figures. |
| 6 | Please show the crystal structures of A, B, and C type GB in main text. The Fig. 10 in appendix is hard to understand. | We will do that. |

#Reviewer 2:

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| No. | Comment | Response |
| 1 | The main reason for a concern is the used method of GB preparation. Here, I can point to three different possible sources of inaccuracy at GB simulation: A) First of all, the authors simulated strongly deformed structure in the bulk part of the calculation cell due to non-equilibrium lattice parameters. At the same time, they used equilibrium value of cohesion energy E0 in eq. (1). It should result in some error at the calculation of GB energy. B) The authors did not describe the minimization procedure for search of the equilibrium configuration of GB. The most common way is the "gamma-surface" method where one grain (i.e. half of the simulated system) is shifted along the GB plane in search of the position with the minimal energy. If the authors used such procedure, they should describe it. C) At consideration of some GB, "gamma-surface" method cannot give equilibrium ordered structure due to formation of defects inside the created GB. This happens when the average atomic density near the GB is different from the bulk. One of the possible methods to find the equilibrium structure of GB is the evolutionary algorithm [T. Frolov, W. Setyawan et al. Grain boundary phases in bcc metals, Nanoscale (2018)]. The other way is MD annealing with the open surface that should be used for creation of the equilibrium GB structure. The use of the open surface in such MD simulation is mandatory aspect as this surface is necessary for formation/removal of GB defects (for instance, see [T. Frolov, Y. Mishin, Phys. Rev. B 79 (2009)] or [S. Starikov, M Mrovec, R Drautz, Acta Materialia 188 (2020)]). Based on the comments given above I strongly recommend the authors to take a step back and to perform the validation of the GB construction method (at least, for several types of GB). | Thank you for your valuable comments:   1. In order to calculate the periodic boundary dimension of the GB system, we have only then considered non-equilibrium lattice constant. During determining E0 in eqn 1 (energy of the pristine crystal), we have considered equilibrated lattice constant. Also, if the non-equilibrated lattice constant (3, 6, 5) is used then after relaxing for 200ps in a NPT ensemble, atomic volume results in 20.8 A3 at 500 K while using the equilibrated lattice constant it is again found as 20.8 A3. In a recent study ( Beeler et at. 2020) this atomic volume at 500 K is observed as 20.5 A3 by AIMD calculation. 2. In page 5, lines 11-15, method to find the equilibrated GB is described. We did not utilize ‘gamma- surface’ method. 3. For each GB, we have considered different simulation box dimensions (both GB area and number of total atoms were varied) to identify size effect on the GB energy. During these operations, always longest dimension in GB plane is kept maximum one-fourth of the simulation box length while maintaining the periodic boundary condition. Also, two boundaries generated within simulation box are kept similar. |
| 2 | The authors used the potential (ADP) developed in 2015. Are there some special reasons explaining why the authors did not use more recent version of this potential [S. Starikov, L. Kolotova, A. Kuksin et al. JNM (2018)]? | Thank you for your response. We have utilized the ADP developed in 2018 (S. Starikov, L. Kolotova, A. Kuksin, D. Smirnova, V. Tseplyaev, Atomistic simulation of cubic and tetragonal phases of u-mo alloy: Structure and thermodynamic properties, Journal of Nuclear Materials 499 (2018)). Unfortunately, we put the wrong reference. |
| 3 | It would be interesting to add more detailed discussion about twins. There are several experimental works about twinning in alpha-uranium [18-20]. The authors only mentioned these works in the Introduction without detailed comparison with the simulation results in the main part of the work. I guess such comparison may add value to this work. | Thank you for your valuable feedback. Unfortunately, the GBs we have studied here, do not describe the experimentally observed twins. Hence, we could only provide a insight on some new probable twins, rather than an explicit comparison. But we will study additional temperature effect on those twins (observed from the current work) . |