Reviewer 1

1. Page 3, paragraph 2: Authors denote possible positions of Xe substitutional atoms in U3Si2 lattice as 2a-U1, 4h-U2, 4g-Si. These notations are used throughout the paper, for example in tables 1 and 4. Please, could you provide an illustration explaining the exact positions of these defects inU3Si2 lattice and the difference between 2a-U1 and 4h-U2 lattice sites?

A figure has been added denoting the unique sites within the U3Si2 crystal.

2. In addition to the potential parameters given in tables 2 and 3, it would be better to add a figure with the plotted potential functions for U-Si-Xe system. Such a picture will give guidance for restoring the potential. It would be especially useful since the original Authors` article describing U-Si potential also had no illustration of the potential functions.

A figure showing the U-Si, U-Xe and Si-Xe pair potentials has been included.

3. Figure 1: I ask Authors to improve the representation of the data in this figure. For this purpose, it would be useful to add an insert showing results for the volumes between 20 and 60 cc/mol. The figure in its current state does not explain clearly the accuracy of representation for pressures P > 1000 MPa. The same comment can be applied to figure 4.

An insert for high pressures has been included in this Figure and in Figure 4.

4. Page 10, last paragraph: Authors discuss relations between the segregation energies attributed to the different grain boundary orientations: GB (210) and GB (730). However, the absolute values of the energies are not given, and the cited paper [44] is currently unpublished (i.e. unavailable). Please provide the absolute values of energies, so the comparison would be evident.

The cited paper has been published. The grain boundary energies are also included in the text for completeness.

Reviewer 2

For the study of the Xe EOS, it will be useful to specify the maximum density of Xe introduced for each size bubble and justify this limit. At least, specify the range of densities studied.

The following text has been added to the manuscript:

“A maximum Xe density inside the bubbles of 30 cc/mol is achieved, corresponding to a pressure of approximately 2 GPa. Bubble pressures in UO2 are only expected to reach GPa for sub-nm radius bubbles, and no such information on bubble pressures in U-Si fuels exists. As such, the pressures investigated in this work span the entire regime of low to high pressure bubbles anticipated in U-Si fuels.”

Do the authors have checked the Xe partial radial distribution function. Is there any structural change as the density of Xe increases in bubble? If not, the EOS equation could change.

The following text has been added to the manuscript:

“The Xe radial distribution has also been analyzed as a function of density. Xe at high pressures and temperatures retain a gas-like radial distribution function, while Xe at high pressures and low temperatures close to the critical point (290 K) begin to exhibit a liquid-like radial distribution function. This generally corresponds to what is expected from the phase diagram.”

Is there any damage appearing on the U3Si2 matrix with the higher Xe density?

The following text has been added to the manuscript:

“Lattice deformation begins to take place around the bubble at very high pressures, but this deformation is minimal and very localized. Previous studies of highly pressurized Xe bubbles in U-Mo showed dislocation ejection from bubbles, however no such phenomenon was observed in this work.”