# The effect of temperature on the calculated bulk vacancy formation energy in Al and Cu

**C. van der Walt, HC Swart and JJ Terblans**
Department of Physics, University of the Free State, PO Box 339, Bloemfontein, South Africa

E-mail address: terblansjj@ufs.ac.za

**To be corrected**
submitted on *Wed 12 Nov 2014 at 16:48*
**Answers**
Does the article you are being asked to review match your expertise? (On scale, + for yes / agree): Neutral
Are there any potential conflicts of interest if you review this article? (+3 for yes / -3 for no): Neutral
A1 Scientific merit: notably scientific rigour, accuracy and correctness: Neutral
A2 Clarity of expression; communication of ideas; readability and discussion of Concepts: Neutral
A3 Sufficient discussion of the context of the work, and suitable referencing: Neutral
B1 Originality: Is the work relevant and novel?: Neutral
B2 Motivation: Does the problem considered have a sound motivation? All papers should clearly demonstrate the scientific interest of the results: Neutral
C1 Title: Is it adequate and appropriate for the content of the article?: Neutral
C2 Abstract: Does it contain the essential information of the article? Is it complete?: Neutral
C3 Diagrams, figures, tables and captions: Are they essential and clear?: Neutral
C4 Text and mathematics: Are they brief but still clear? If you recommend shortening, please suggest (below at comments) what should be omitted: Neutral
C5 Conclusion: Does the paper contain a carefully written conclusion, summarising what has been learned and why it is interesting and useful?: Neutral

**Reply**

Corrected

**REJECTED**
submitted on *Mon 10 Nov 2014 at 18:19*

**Comments**

The authors study effects of temperature on the calculated bulk vacancy formation energy in Al and Cu by using the embedded atom method, with the potential developed by Sutton and Chen. The method is well know. See, for example the series

of publications by J.I. Akhter, and the references therein.
In the present study the authors appear to have combined their results from two previous papers (References 1 and 2 in the manuscript) into the present article. There is nothing novel about the present calculation, other than the fact that a different number of atoms was used for the simulation (about 600 in Refs. 1 and 2, as opposed to 1994 in the present work). Thus the small differences seen in the results may be attributed to the different numbers of atoms employed in the simulations. The article makes no attempt to compare whether the larger simulation domain brings us any closer to the experimentally observed values. Furthermore, the authors do not provide essential information about the numerical aspects of the computation, such whether or not they are using their own code, integration algorithm used, the time step, cut-off radius, etc. Therefore it is difficult to say whether or not the simulated results might be inaccurate due to, for example, a lack of equilibration, or size effects. However, irrespective of these obvious deficiencies, there seems to be nothing new about the present article, and it should be rejected for this reason alone.

**Criteria Evaluation**
Does the article you are being asked to review match your expertise? (On scale, + for yes / agree): Strongly Agree
Are there any potential conflicts of interest if you review this article? (+3 for yes / -3 for no): Strongly Disagree
A1 Scientific merit: notably scientific rigour, accuracy and correctness: Neutral
A2 Clarity of expression; communication of ideas; readability and discussion of Concepts: Neutral
A3 Sufficient discussion of the context of the work, and suitable referencing: Neutral
B1 Originality: Is the work relevant and novel?: Neutral
B2 Motivation: Does the problem considered have a sound motivation? All papers should clearly demonstrate the scientific interest of the results: Neutral
C1 Title: Is it adequate and appropriate for the content of the article?: Neutral
C2 Abstract: Does it contain the essential information of the article? Is it complete?: Neutral
C3 Diagrams, figures, tables and captions: Are they essential and clear?: Neutral
C4 Text and mathematics: Are they brief but still clear? If you recommend shortening, please suggest (below at comments) what should be omitted: Neutral
C5 Conclusion: Does the paper contain a carefully written conclusion, summarising what has been learned and why it is interesting and useful?: Neutral

**Reply**

Clarifying the code is new and the advantages of using said code above quantum mechanics calculations

Included new details concerning thermostat, integration method and requested constants used.

Added comment clarifying cause of error spread

**ACCEPTED**

submitted on *Mon 10 Nov 2014 at 18:18*

**Comments**

The authors use the embedded atom potential to study atomic vacancies in Al and Cu using a molecular dynamics scheme. This method has been superseded by modern quantum mechanical methods. Nevertheless, the novel aspect of their work is to include the effects of temperature. The motivation for this work is not sufficiently well articulated. I recommend publication in the proceedings of the SAIP.

**Criteria Evaluation**

Does the article you are being asked to review match your expertise? (On scale, + for yes / agree): Strongly Agree
Are there any potential conflicts of interest if you review this article? (+3 for yes / -3 for no): Strongly Disagree
A1 Scientific merit: notably scientific rigour, accuracy and correctness: Neutral
A2 Clarity of expression; communication of ideas; readability and discussion of Concepts: Agree
A3 Sufficient discussion of the context of the work, and suitable referencing: Agree
B1 Originality: Is the work relevant and novel?: Neutral
B2 Motivation: Does the problem considered have a sound motivation? All papers should clearly demonstrate the scientific interest of the results: Neutral
C1 Title: Is it adequate and appropriate for the content of the article?: Agree
C2 Abstract: Does it contain the essential information of the article? Is it complete?: Agree
C3 Diagrams, figures, tables and captions: Are they essential and clear?: Agree
C4 Text and mathematics: Are they brief but still clear? If you recommend shortening, please suggest (below at comments) what should be omitted: Agree
C5 Conclusion: Does the paper contain a carefully written conclusion, summarising what has been learned and why it is interesting and useful?: Neutral