Multiscale Modeling of the Interfacial Fracture Behavior in the Sn–Cu₆Sn₅–Cu System

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With the increasing focus on developing environmentally-benign electronic packages, Pb-free alloys have received a great deal of attention. Mishandling of packages, during manufacture, assembly, or by the user may cause failure of solder joint. Very few reports to-date in the literature have delved into the microstructural mechanisms for fracture in Pb-free solder joints that usually comprising many interfaces between Cu and intermetallic (IMC) layers, as well as IMC and Sn. Such an understanding is necessary for designers to make informed decisions when designing new robust and environmentally-benign electronics packages. In this paper, we have established a cohesive law for IMC and Sn interfaces based on the modified embedded atom methods. By using the continuum homogeneous approach, the interfacial stress/separation relation and the cohesive energy is obtained. The theoretical analysis predicts that the interface has the largest cohesive energy compared with pure Sn and IMC, which explains the reason why the fracture always occurs at the pure Sn instead of the interface. The experiments have been conducted to validate this analysis. This study provides a constitutive relation of IMC/Sn interfaces that can be used to other fracture behavior of Pb-free solder joints, such as under mechanical vibration conditions.

Keywords: Intermetallic (IMC) Materials, Interfaces, Cohesive Energy.

1. INTRODUCTION

With emerging environmental regulations worldwide and an increasing focus on developing environmentally-benign electronic packages, Pb-free solders have received a great deal of attention.1-6 The European Union (EU) Waste Electrical and Electronic Equipment Directive (WEEE) and Restriction of Hazardous Substances Directive (RoHS) have come into effect prohibiting the intentional addition of lead to most consumer electronics produced in the EU. Similar directives have also been passed in the rest of the world.

Most Pb-free solders are Sn-rich, with small alloying additions of Ag, Cu, or both Ag and Cu. The important microstructural features of a typical Sn-rich joint, with composition of Sn-3.9Ag-0.7Cu, are shown in Figure 1. The solder microstructure consists of Sn dendrites decorated by a eutectic mixture of Ag₅Sn and Cu₆Sn₅ intermetallic particles. The solder microstructure, as controlled by cooling rate, inherently controls the mechanical response of the joint.7-10 In addition, a Cu₆Sn₅ intermetallic (IMC) layer grows from the reaction between the Sn-rich liquid (during melting) and the Cu substrate. The thickness and morphology of this IMC layer also significantly affects the mechanical performance of the solder. Because of the difference in thermal expansion between various layers in the package, the solder will be subjected to a myriad of stresses and strains. Indeed, the mechanical behavior of Pb-free alloys is extremely important because solder joints must retain their mechanical integrity under a variety of conditions, such as thermomechanical fatigue, creep, thermal aging, and vibration and mechanical shock. Mishandling of packages, particularly during manufacture and assembly, may also cause failure of solder joint.

Very few reports to-date in the literature have delved into the microstructural mechanisms for fracture in Pb-free solder joints. The fracture mechanisms in Pb-free solder joints are quite complex due to: (a) the large difference in deformation behavior of the individual components, and (b) the many interfaces that are formed in the system. Broadly speaking, the fracture in these joints can be categorized by solder-based fracture or IMC-controlled fracture. Chawla1 notes that the type of fracture is likely a
function of the applied strain rate and the thickness of the IMC layer. Higher strain rates and larger IMC thicknesses favor brittle fracture through the IMC. In many reports, fracture at or within the IMC layer has been observed.11–13 A recent report by Suh et al.11 showed that by decreasing the content of Sn, more plasticity energy dissipation took place that enhanced the drop resistance by over a factor of ten in Sn-1Ag-0.5Cu compared to a conventional Sn-4Ag-0.5Cu. The fracture mode shifted from IMC failure in the higher content Ag material to that of failure within the solder at lower Ag content. Liu et al.12 showed that solder aging decreased the drop resistance of the solder joint, although it is not clear whether this was due to an increase in IMC thickness or a decrease in solder strength. Mattila et al.13 studied the mechanical drop behavior of several solder and metallization combinations. They hypothesized that the main failure mechanism under mechanical shock loading is related to the high deformation rates and strain-rate hardening of the solder which forces cracks to propagate in the IMC layers instead of the bulk solder. Song et al.14 examined the role of microstructure on the vibration fatigue properties of a Sn-rich solder alloy. Coarser eutectic regions with larger β-Sn dendrites contributed to a higher damping capacity and, thus, a greater vibration life. It was postulated that needle-like eutectic Ag₃Sn and large primary Ag₃Sn plates accelerated crack growth and, thus, degraded the ductility and vibration fracture resistance.

A comprehensive understanding of the fracture behavior of Pb-free solder joints requires the application of accurate and realistic constitutive relations for the individual components as well as the behavior of the interfaces. One way to study the interfacial behavior of materials in this system is by molecular simulations (e.g., molecular dynamics using empirical bond order potentials). Molecular simulations, however, are only valid for short time scales (on the order of 10⁻¹² second) and length scales (on the order to 1 µm), so we cannot model the entire solder joint system using this approach. On the other hand, continuum models, especially cohesive zone models have been widely used in the continuum study of interfacial fracture.15–17 A cohesive zone model assumes a cohesive zone law that is described by the relationship between normal traction and the opening displacement of the interface. By using the multi-scale approach, the continuum cohesive law can be extended to the atomic domain. Recently, this approach has been used to develop a cohesive law for the interface between carbon nanotubes and a polymer matrix in polymer composites.18–22

In this paper, we have used a multiscale approach to model the deformation behavior of a Sn/Cu₆Sn₃/Cu system. The cohesive law for the interface between Sn and Cu₆Sn₃ was obtained from a modified embedded atom method (MEAM). Finite element analysis was then conducted, with the appropriate stress–strain constitutive behavior for the individual components, i.e., Sn, Cu₆Sn₃, and Cu. We begin by briefly reviewing the MEAM and how one can apply it to the interface between Sn and Cu₆Sn₃. In the next sections, we describe the cohesive law and finite element simulations that incorporate the cohesive law. We conclude with a comparison to experiments on Pb-free solder joints and fractographic analysis.
2. APPLICATION OF THE MODIFIED EMBEDDED ATOM METHOD (MEAM) TO Sn/Cu₅Sn₅ INTERFACE

In this section we briefly review the MEAM potential and its application to determining the stress-strain behavior of the interface between Sn and Cu₅Sn₅. A detailed discussion of the potential can be found elsewhere. The total energy, \( U \), of an embedding atom \( A \) into a sea of "background atoms" \( B \) is given by (Fig. 2):

\[
U = \sum_i F_A(\rho_{i,AB}) + \frac{1}{2} \sum_{i<j} \phi_{AB}(R_{ij})
\]

where \( i \) and \( j \) denote the spatial positions for type \( A \) atoms and type \( B \) atoms, respectively. \( F_A \) is the embedding function of the type \( A \) atom and is a function of the local electron density \( \rho_{i,AB} \) given by the background atoms \( B \). \( F_A \) is given by the following expression:

\[
F_A = A_ag\phi_A^0 \ln \rho_{i,AB}
\]

where \( A_a \) is a dimensionless adjustable parameter and \( g\phi_A^0 \) is the cohesive energy of atom type \( A \). The local electron density \( \rho_{i,AB} \) encompasses the total contributions from all background atoms \( B \) to the embedding atom \( A \) at position \( i \). This function decays with an increase in distance between atoms \( A \) and \( B \), which is given by:

\[
\rho_{i,AB} = \sum_j \exp\left[-\beta_B \left( \frac{R_{ij}}{R_{AB}} - 1 \right) \right]
\]

where \( \beta_B \) is a decay constant and \( R_{AB}^0 \) is the equilibrium distance between nearest neighboring atoms in the reference lattice (i.e., a conceptual material comprising atoms \( A \) and \( B \) with a ratio of their valences). Function \( \phi_{AB} \) is the pair potential between two atoms of type \( A \) and \( B \) and depends on the interatomic distance \( R_{ij} \). It is noted that the embedding atom and the background atom can be the same or different since one can embed a pure metal into an alloy that has the composition of the metal as we will discuss in the following.

In our system, we are interested in the interface between Sn and Cu₅Sn₅. Thus, the interface between IMC and pure Sn involves embedding Cu and Sn atoms, with a ratio of 6:5, into the Sn background. The local electron density of a Cu atom is \( \rho_{i,Cu} = \sum_j \exp\left[-\beta_{Sn} \left( \frac{R_{ij}}{R_{Cu,Sn}^0} - 1 \right) \right] \) by taking a Cu-Sn alloy with ratio of 3:1. It should be noted that Cu₅Sn (by the ratio of valences of Cu and Sn) is taken as the reference, although Cu₅Sn is not the really alloy here, and \( R_{Cu,Sn}^0 \) is taken as the average lattice constant in Cu₅Sn. The local electron density for a Sn atom is \( \rho_{i,Sn} = \sum_j \exp\left[-\beta_{Sn} \left( \frac{R_{ij}}{R_{Sn}^0} - 1 \right) \right] \). The pair potential for two Sn atoms is then given by:

\[
\phi_{Sn-Sn}(R_{ij}) = \frac{1}{2} \left[ -E_{Sn}^0 \left( 1 + \alpha_{Sn} \left( \frac{R_{ij}}{R_{Sn}^0} - 1 \right) \right) \right] \times \exp\left[ -\alpha_{Sn} \left( \frac{R_{ij}}{R_{Sn}^0} - 1 \right) \right] - F_{Sn} \left( \frac{\rho_{i,Sn}}{4} \right)
\]

and the counterpart potential for a Cu atom and a Sn atom is:

\[
\phi_{Cu-Sn}(R_{ij}) = -\frac{1}{3} E_{Cu,Sn}^0 \left( 1 + \alpha_{Cu,Sn} \left( \frac{R_{ij}}{R_{Cu,Sn}^0} - 1 \right) \right) \times \exp\left[ -\alpha_{Cu,Sn} \left( \frac{R_{ij}}{R_{Cu,Sn}^0} - 1 \right) \right] - \frac{1}{4} F_{Cu} \left( \frac{\rho_{i,Cu}}{12} \right) - \frac{1}{6} F_{Cu} \left( \frac{\rho_{i,Sn}}{12} \right)
\]

The parameters used are listed in Table I.

### Table I. Parameters of MEAM potential for the interface between Sn and Cu₅Sn₅.

<table>
<thead>
<tr>
<th>Composition</th>
<th>( E_a^0 ) (eV)</th>
<th>( A )</th>
<th>( R_0^0 ) (nm)</th>
<th>( \alpha )</th>
<th>( \beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>3.62</td>
<td>1.07</td>
<td>0.25</td>
<td>5.106</td>
<td>3.62</td>
</tr>
<tr>
<td>Sn</td>
<td>3.08</td>
<td>1.0</td>
<td>0.344</td>
<td>6.20</td>
<td>6.2</td>
</tr>
<tr>
<td>Cu₅Sn</td>
<td>3.5</td>
<td>0.268</td>
<td>0.538</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3. THE COHESIVE LAW FOR Pb-FREE SOLDER JOINTS

Using the MEAM results as a basis, we can now formulate the cohesive law for the Sn/Cu₅Sn₅ interface in the system. It should be noted that fracture in Sn–Cu joints almost always takes place within the solder, in the vicinity of the...
Sn/Cu₆Sn₅ IMC layer, or within the IMC layer. Since fracture never really takes place between Cu and Cu₆Sn₅, we assume perfect bonding at this interface. Atomic structures of Cu (FCC), IMC, and Sn (BCT) are needed to calculate the number densities of atoms to be used in the analysis and the interface is illustrated in Figure 3.

3.1. One Layer IMC/Sn

We first consider the interaction of one layer of IMC atoms and Sn (Fig. 4), i.e., the interaction between the IMC and Sn is limited to the nearest neighboring IMC atoms. The separation distance between the IMC layer and Sn is represented by \( h \) (which is to be determined). The energy stored in an infinitesimal area \( d\Omega \) of the IMC layer can be written as:

\[
U = \sum_{i \text{ of } \text{Sn in } d\Omega} \left[ F_{\text{Sn}}(\vec{p}_{i,\text{Sn}}) + \frac{1}{2} \sum_{j \text{ of bulk Sn}} \phi_{\text{Sn-Sn}}(R_{ij}) \right] \\
+ \sum_{i \text{ of Cu in } d\Omega} \left[ F_{\text{Cu}}(\vec{p}_{i,\text{Cu}}) + \frac{1}{2} \sum_{j \text{ of bulk Sn}} \phi_{\text{Cu-Sn}}(R_{ij}) \right]
\]

(6)

Instead of using a discrete summation over all Cu and Sn atoms, we adopt a continuum method by homogenization. Specifically, the discrete summation is evaluated by means of integration. Equation (6) then becomes:

\[
U = \rho_{\text{Sn}}^{\text{IMC}} \tau_{\text{IMC}} d\Omega \left[ F_{\text{Sn}}(\vec{p}_{\text{Sn}}) + \frac{1}{2} \int_{V_{\text{bulk Sn}}} \phi_{\text{Sn-Sn}}(R) \rho_{\text{Sn}}^{\text{bulk}} dV \right] \\
+ \rho_{\text{Cu}}^{\text{IMC}} \tau_{\text{IMC}} d\Omega \left[ F_{\text{Cu}}(\vec{p}_{\text{Cu}}) + \frac{1}{2} \int_{V_{\text{bulk Sn}}} \phi_{\text{Cu-Sn}}(R) \rho_{\text{Sn}}^{\text{bulk}} dV \right]
\]

(7)

where \( \rho_{\text{Cu}}^{\text{IMC}} = 26.76 \text{ (nm}^3) \) and \( \rho_{\text{Sn}}^{\text{IMC}} = 22.3 \text{ (nm}^3) \) are number densities of Sn and Cu atoms in the IMC; \( \tau_{\text{IMC}} = 1/3(a_{\text{IMC}} + b_{\text{IMC}} + c_{\text{IMC}}) = 0.45 \text{ nm} \) is the average thickness of an IMC layer; \( V_{\text{bulk Sn}} \) is the volume of the bulk Sn as the background; and \( \rho_{\text{Sn}}^{\text{bulk}} = 34 \text{ (nm}^3) \) is the number density of Sn atom in the bulk Sn. The subscripts “i” and “j” for local electron density \( \vec{p} \) and distance \( R \) are dropped since for the infinite two-dimensional layer and three-dimensional bulk, specific positions are not important in the infinite body.

The local electron density can also be evaluated by integration over all background Sn atoms. The distance between a point \((x, y)\) on the IMC layer and a point \((z, r)\) \((z \geq h, \ r \geq 0)\) in the bulk Sn (Fig. 4) is \( R_{ij} = \sqrt{r^2 + z^2} \). Then, the local electron densities can be expressed and obtained as:

\[
\vec{p}_{\text{Cu}} = \int_{z=h}^{\infty} \int_{r=0}^{\infty} -\beta_{\text{Sn}} \left( \frac{\sqrt{r^2 + z^2}}{R_{\text{Cu-Sn}}} - 1 \right) \rho_{\text{Sn}}^{\text{bulk}} 2\pi r dr dz \\
= 2\pi \rho_{\text{Sn}}^{\text{bulk}} h \left( \frac{R_{\text{Cu-Sn}}^0}{\beta_{\text{Sn}}^3} \right) \left( \beta_{\text{Sn}} + \frac{2R_{\text{Cu-Sn}}^0}{h} \right) \\
\times \exp \left[ -\beta_{\text{Sn}} \left( 1 - \frac{h}{R_{\text{Cu-Sn}}^0} \right) \right] \tag{8}
\]

\[
\vec{p}_{\text{Sn}} = \int_{z=h}^{\infty} \int_{r=0}^{\infty} -\beta_{\text{Cu}} \left( \frac{\sqrt{r^2 + z^2}}{R_{\text{Sn-Sn}}} - 1 \right) \rho_{\text{Sn}}^{\text{bulk}} 2\pi r dr dz \\
= 2\pi \rho_{\text{Sn}}^{\text{bulk}} h \left( \frac{R_{\text{Sn-Sn}}^0}{\beta_{\text{Sn}}^3} \right) \left( \beta_{\text{Sn}} + \frac{2R_{\text{Cu-Sn}}^0}{h} \right) \\
\times \exp \left[ -\beta_{\text{Sn}} \left( 1 - \frac{h}{R_{\text{Sn}}^0} \right) \right] \tag{9}
\]

The analytical expressions for the pair potential can also be obtained, although it is somewhat lengthy (see Appendix). The above expressions all depend on a single variable, the separation distance \( h \). The cohesive energy \( \Phi \) is the energy per unit volume and is given by:

\[
\Phi(h) = \frac{U(h)}{\tau_{\text{IMC}} d\Omega} \tag{10}
\]

The equilibrium separation between a single layer of IMC and a bulk Sn is determined by the minimization of the cohesive energy with respect to the separation \( h \), i.e., to solve \( h \) via

\[
\frac{\partial \Phi}{\partial h} = 0 \tag{11}
\]

and

\[
h = h_0 = 0.297 \text{ nm} \tag{12}
\]

Upon external load, the separation deviates from the equilibrium separation \( h_0 \) to \( h_0 + \Delta h \), where \( \Delta h \) is the increment or opening displacement. Thus, the cohesive energy depends on the opening displacement \( \Delta h \), i.e., \( \Phi = \Phi(h_0 + \Delta h) \), by simply replacing \( h \) to \( h_0 + \Delta h \). Note that the
sliding displacement does not affect the cohesive energy because of the infinite size of the two-dimensional layer and three-dimensional plate. This leads to the shear cohesive stress being negligible. The tensile cohesive stress is the obtained from the work-conjugate relation by:

\[ \sigma(\Delta h) = \frac{\partial \Phi(\Delta h)}{\partial (\Delta h/h_0)} \]  

Equation (13) gives the cohesive law for one layer of IMC and bulk Sn, as shown in Figure 5. The cohesive strength is given by \( \sigma_{\text{max}} = 12.67 \) GPa and is reached at the critical separation distance, \( \Delta h_{\text{critical}} = 0.062 \) nm. The area under the curve represents the total cohesive energy and is \( \Gamma = 2.22 \) J/m².

3.2. Multiple Atomic Layers of IMC on Sn

Now we consider multiple atomic layers of IMCs interacting with bulk Sn (Fig. 6). The interactions between IMC layers are ignored in the following analysis. In other words, IMC layers are separated from the bulk Sn as a whole, which provides an upper-limit of the interfacial strength. The interlayer spacing of the IMC layers is taken to be the average IMC lattice constants \( a_{\text{IMC}}, b_{\text{IMC}} \) and \( c_{\text{IMC}} \) by \( t_{\text{IMC}} = 1/(a_{\text{IMC}} + b_{\text{IMC}} + c_{\text{IMC}}) = 0.45 \) nm. The total cohesive energy \( \Phi_{\text{multi-layer}} \) is then given by:

\[ \Phi_{\text{multi-layer}}(h) = \Phi(h) + \Phi(h + t_{\text{IMC}}) + \cdots + \Phi(h + nt_{\text{IMC}}) \]  

where \( \Phi(h) \) is the cohesive energy for the single layer of IMC/bulk Sn, given by Eq. (10); \( n + 1 \) is the number of IMC layers. The expression for each term on the right hand side of Eq. (14) is the same as that given by Eq. (10) if \( h \) is replaced by \( h + t_{\text{IMC}} \). The equilibrium separation is then determined by energy minimization with respect to \( h \) for a given layer of \( n \) (i.e., \( n \geq 1 \))

\[ h = h_0 \approx 0.296 \text{ nm}, \quad n \geq 1 \]  

4. FINITE ELEMENT ANALYSIS AND COMPARISON WITH EXPERIMENTS

The very high cohesive energy of the interface between IMC and Sn may explain why fracture, experimentally, occurs in bulk Sn, instead of the strong IMC/Sn interface. The cohesive energy provides the fracture resistance based on the Griffith energy balance. The cohesive energies for pure Sn and IMC have been given either by experiments or atomic simulations. The typical value for Sn\textsuperscript{27} is 0.681 J/m² and for Cu\textsuperscript{27} 1.031 J/m², which are much smaller than the cohesive energy \( \Gamma = 2.22 \) J/m² for the interface as predicted by this analysis. It should be noted that fracture in ductile materials, such as Cu and Sn, takes...
place by slip, void growth, etc., so fracture will take place at a stress much lower than the cohesive strength.

In order to validate our theoretical analysis, we compare with experiments by finite element analysis. Cylindrical samples, consisting of a thin Sn section sandwiched between two copper bars, were tested in tension. The dimension and the geometry of the joint are illustrated by Figure 7. The strain was measured by extensometer with a 10 mm gage length. Most of the strain comes from the plastic deformation of the Sn, but the elastic contribution of the Cu bars was also substracted.

The finite element model consisted of Cu, IMC, interface and bulk Sn. Cu is modeled as an elastic material with Young’s modulus of 116 GPa and Poisson’s ratio of 0.3. IMC had a Young’s modulus of 112.3 GPa and Poisson’s ratio of 0.3. Pure Sn was modeled as an elastic-plastic material and was determined by experiments on bulk Sn. The stress-separation constitutive relation of IMC/Sn interface is given by Eq. (13) or Figure 5. The same geometry and compensation are used to compare with experiments. The thickness of interface is taken to be 0.01 mm in the simulation. We used CAX4H axisymmetric elements in ABAQUS finite element analysis package. Model convergence was reached by continuously refining the mesh until the values of stress did not change. Figure 8 shows the von-Misses stress and the effective plastic strain, in which it is noted that the maximum stress/strain takes place at Sn very close to IMC. This is another piece of evidence that the fracture always occurs at the bulk Sn near to the interface between IMC and Sn.

Figure 9 shows the stress and strain curve for both experiments and theoretical analysis. A fairly good agreement between experiment and simulation is observed. The simulation curve increases continuously, while the experiment decreases more quickly. This can be attributed to the fact that a fracture criterion in the solder was not used, and that in the experiment fracture takes place by void growth in the Sn. These voids are nucleated by the nodular morphology of the IMC layer. A typical fracture surface is shown in Figure 10. Note that the nodules of Cu$_6$Sn$_5$ are at the base of the voids.

![Fig. 8. Finite element results of the effective stress and strain contours for a Pb-free solder joint subject to uniaxial tension.](image1)

![Fig. 9. Stress-strain curve for a Pb-free solder joint subject to uniaxial tension for both theoretical analysis and experiments.](image2)

![Fig. 10. Fractographic images of IMC.](image3)
5. CONCLUSION REMARKS

We have obtained the cohesive law for IMC and Sn interfaces based on the modified embedded atom methods. By using the continuum homogeneous approach, the interfacial stress/separation relation and the cohesive energy is obtained. The theoretical analysis predicts that the interface has the largest cohesive energy compared with pure Sn and IMC, which explains the reason why the fracture always occurs at the pure Sn instead of the interface. The experiments have been conducted to validate this analysis. This study provides a constitutive relation of IMC/Sn interfaces that can be used to other fracture behavior of Pb-free solder joints, such as under mechanical vibration conditions.

APPENDIX

The integration of pair potential over the volume of the bulk Sn can be expressed by a double integration as follows:

\[
\frac{1}{2} \int_{V_{\text{bulk-Sn}}} \phi_{\text{Sn-Sn}}(R) \rho_{\text{Sn}}^{\text{bulk}} \, dV
\]

\[
= \frac{1}{2} \int_{r=0}^{\infty} \int_{0}^{\infty} \phi_{\text{Sn-Sn}}(R) \rho_{\text{Sn}}^{\text{bulk}} 2 \pi r \, dr \, dz
\]

\[
= \frac{1}{2} \pi \rho_{\text{Sn}}^{\text{bulk}} \frac{R_{\text{Sn}}^{0} h^{2} E_{\text{Sn}}^{0}}{(\alpha_{\text{Sn}})^{3}} \exp \left[ \frac{\alpha_{\text{Sn}}}{(1 - h/R_{\text{Sn}}^{0})} \right] \times \left[ -(\alpha_{\text{Sn}})^{2} - \frac{5 R_{\text{Cu}}^{0} \alpha_{\text{Cu}}}{h} + \frac{R_{\text{Cu}}^{0} (\alpha_{\text{Cu}})^{2}}{h} \right] \times \left[ -8 \left( \frac{R_{\text{Cu}}^{0}}{h} \right)^{2} + 2 \alpha_{\text{Cu}} \left( \frac{R_{\text{Cu}}^{0}}{h} \right)^{2} \right] \times \left[ -\beta_{\text{Sn}}^{2} \frac{4 R_{\text{Sn}}^{0} \beta_{\text{Sn}}}{h} + \frac{R_{\text{Sn}}^{0} \beta_{\text{Sn}}}{h} \right] \times \left[ -6 \left( \frac{R_{\text{Sn}}^{0}}{h} \right)^{2} + 2 \beta_{\text{Sn}} \left( \frac{R_{\text{Sn}}^{0}}{h} \right)^{2} \right]
\]

\[
= \frac{1}{2} \int_{V_{\text{bulk-Sn}}} \phi_{\text{Cu-Sn}}(R) \rho_{\text{Sn}}^{\text{bulk}} \, dV
\]

\[
= \frac{1}{2} \int_{r=0}^{\infty} \int_{0}^{\infty} \phi_{\text{Cu-Sn}}(R) \rho_{\text{Sn}}^{\text{bulk}} 2 \pi r \, dr \, dz
\]

\[
= \frac{1}{2} \pi \rho_{\text{Sn}}^{\text{bulk}} \frac{R_{\text{Cu}}^{0} h^{2} E_{\text{Cu}}^{0}}{(\alpha_{\text{Cu}})^{3}} \exp \left[ \frac{\alpha_{\text{Cu}}}{(1 - h/R_{\text{Cu}}^{0})} \right] \times \left[ -(\alpha_{\text{Cu}})^{2} - \frac{5 R_{\text{Cu}}^{0} \alpha_{\text{Cu}}}{h} + \frac{R_{\text{Cu}}^{0} (\alpha_{\text{Cu}})^{2}}{h} \right] \times \left[ -8 \left( \frac{R_{\text{Cu}}^{0}}{h} \right)^{2} + 2 \alpha_{\text{Cu}} \left( \frac{R_{\text{Cu}}^{0}}{h} \right)^{2} \right] \times \left[ -\beta_{\text{Cu}}^{2} \frac{4 R_{\text{Cu}}^{0} \beta_{\text{Cu}}}{h} + \frac{R_{\text{Cu}}^{0} \beta_{\text{Cu}}}{h} \right] \times \left[ -6 \left( \frac{R_{\text{Cu}}^{0}}{h} \right)^{2} + 2 \beta_{\text{Cu}} \left( \frac{R_{\text{Cu}}^{0}}{h} \right)^{2} \right]
\]

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