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Modeling and Simulation – The Effects of Grain Coarsening on Local Stresses and Strains in Solder Microstructure

By

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ABSTRACT

A critical issue in the long-term reliability of solder connections used in electronic packages is the joint failure during thermal cycling. Presently in most finite element analysis to predict the solder joint fatigue failures, solder is assumed as a homogeneous single-phase metal. However in the last decade, several metallurgical studies have shown that solder microstructure may have a role in early solder joint failures (ref 1). Investigators have observed (ref 1) that solder microstructure coarsens in local bands during aging and during thermal cycle fatigue. In a failed solder joint, the fatigue cracks are found in these bands of coarse grains. It is speculated that the grain coarsening increases the local strains within the microstructure, thereby increasing the likelihood for a crack to initiate. The objective of this study is to model and simulate the effect of grain coarsening on local stresses and strains.

During solidification of eutectic Pb/Sn solder, two types of microstructures form, namely lamellar and equiaxed. In this study, I have developed a computer code to generate both types of microstructures of varying grain coarseness. This code is incorporated into the finite element (FE) code that analyzes the local stresses and strains within the computer-generated microstructure. The FE code, specifically developed for this study, uses an algorithm involving the sparse matrix and iterative solver. This code on a typical single-processor machine will allow the analyst to use over 1 million degrees of freedom. For higher number of degrees of freedom, we have also developed a code to run on a parallel machine using message passing interface. The data reported in this paper were obtained using the single-processor code.The solder microstructure, if assumed to be homogeneous single phase, has gradual variation in local stresses and strains. In 2-phase solder, von mises stresses and strains are heterogeneously distributed. In general, the maximum von mises stress in 2-phase solder case are higher than in 1-phase solder. In lamellar microstructure of 2-phase solder, the maximum von mises stress in the microstructure gradually increases with grain coarseness. In equiaxed microstructure of 2-phase solder, the maximum von mises stress does not follow a general trend, increasing or decreasing, with increasing grain coarseness.

1. Background

In electronic assemblies, solder joints are used to obtain electrical, thermal and mechanical connection between the electronic component and the printed wiring board . Solder joint reliability is a major concern in these assemblies and is likely to become even more critical in the future circuits, which will have denser circuitry and will be required to have higher performance. A crucial issue in the long-term reliability of solder joints is the joint failure during thermal cycling.

A packaging engineer typically does thermal-mechanical modeling assuming solder as a homogeneous body. In reality, solder microstructure is highly heterogeneous, involving Pb-rich, Sn-rich and intermetallic phases. In the last decade, several metallurgical studies have shown that solder microstructure may have a role in early solder joint failures (ref 1). The morphology of solder microstructure depends on its processing history, and evolves in a complex way during aging and thermal cycling. It has been suggested that microstructure of solder coarsens in local bands during aging and thermal-mechanical cycling. The analysis of failed solder joints have shown that the failure cracks are found within the band of coarser grains (ref. 1). The mechanisms for the reduced solder joint reliability caused by grain coarsening are not well understood. There

is a need to get parametric insight into the solder joint weakening due to microstructure coarsening. Modeling and simulation is a cost effective way to conduct such a study.

2. Objective of the Study

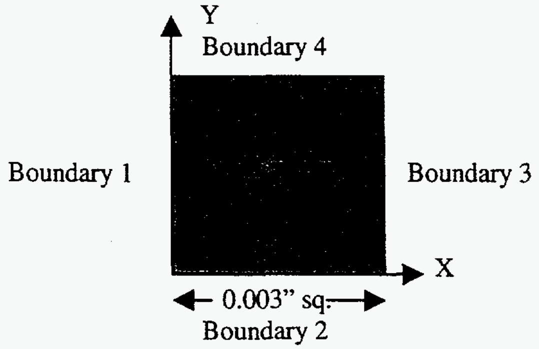
The goal of the present study is to model and simulate the effects of microstructure coarsening on the stresses and strains within the solder microstructure. The actual stress and strain state of the microstructure is far more complex than the elastic model used in this study. However, from the elastic model, we can calculate von mises stresses. Von mises stresses provide yield criteria, i. e. the solder would yield and plastically deform if Von mises stress exceeds yield strength. The plastic strains, which cause fatigue failures in solders, are proportional to von mises stress values exceeding yield strength.

The tasks to accomplish the goal of the study are:

1) Define the problem for finite element analysis.
2) Develop a code to generate microstructure.
3) Develop the finite element code.
4) Conduct parametric study of the eutectic solder microstructure.

3. Definition of the Problem

The problem definition is as follows.



Boundary Conditions

The boundary condition is chosen such that displacement of the solder joint in BGA occurs only in x direction on boundaries 2 and 4. Thermal expansivity of silicon is 3 ppm/°K and that of printed wiring board is 20 ppm/°K. Taking the most extreme example of bare silicon, 1" sq, attached to the printed wiring board with solder balls, for a thermal excursion of 200°C, we can expect to see thermal expansion of (+0.001)*L on boundary 4 and (-0.001)*L on boundary 2 in x—direction, L being the domain length.

Boundary 1: Free

Boundary 2:

$Ux = -0.000003$

$Uy = 0$

Boundary 3: Free

Boundary 4:

$Ux = +0.000003$

$Uy = 0$

Governing Equation

$\delta \sigma_{ij} / \delta X_j = 0$

where σ_{ij} = stress in ith plane in j-direction

X_j = displacement in jth direction

Constitutive Equation

$\sigma_{ij} = 2*\mu*\varepsilon_{ij} + \lambda*\varepsilon_{kk}*\delta_{ij}$

where $2*\mu = E / (1 - \upsilon)$

$\lambda = \upsilon*E/((1+\upsilon)*(1-2*\upsilon))$

E = young's modulus

υ = poisson's ratio

Assumptions Made in the Model

The following assumptions were made about the microstructure in the model.

1. The grain/domains are square.
2. The displacement is in x-direction only.
3. Only eutectic solder has been considered.
4. Sn-rich and Pb-rich are the two major phases in eutectic solders. The composition of these two phases are very close to that of pure metals. Thus, I have assumed that Sn-rich and Pb-rich are pure Sn and pure Pb.
5. In eutectic solder , 63% Sn & 37% Pb, the volume percent of Sn and Pb are 72% and 28%, respectively. In the model, the assumed volume %s of Sn and Pb are 67% and 33%, respectively. This volume ratio simplifies the computer generated microstructure into having two volumes of Sn for every volume of Pb.

Material properties

The material properties are listed in Table 1.

4. Code to Generate Microstructure

The microstructure is highly dependent on its processing, aging and strain history. For example, when eutectic solder is cooled very slowly from its molten state, a lamellar microstructure develops, as shown in Figure 1. When the cooling is very fast, a fine equiaxed microstructure develops as illustrated in Figure 2. In general, these microstructures coarsen in local bands during aging and cyclic stresses. I have developed a code to generate lamellar and equiaxed microstructure of varying coarseness.

Lamellar Microstructure
The lamellar microstructure was obtained by arranging two stripes of Sn for every stripe of Pb as shown in Figure 3. The coarsening parameter is referred to as coarseness, which is the number of elements per side per grain. Coarseness varies from 1 to 12 when the problem size is 72 elements per side. With higher number of elements per side, higher coarseness numbers are possible.

Equiaxed Microstructure
The equiaxed microstructure was obtained by filling in the solder packets, containing two volumes of Sn for every volume of Pb. The occurance order of Pb or Sn within the packet is determined randomly. This scheme maintained the same local composition in spite of randomness. The example of computer generated equiaxed microstructure is shown in Figure 4 for coarseness of 1 to 12.

5. Finite Element (FE) Code

The major issues in developing a code to run large problems on single processor are the memory and time needed for each run. Both of these issues are dependent on the algorithm chosen. An algorithm using sparse matrix and solving the matrix equation by iterative methods, Gauss Seidel and Jacobi, was developed and coded. A convergence rate of approximately 2 was obtained applying this code to a single-phase solder. The maximum degrees of freedom that we were able to run with this code was over one million. For a larger problem, the code was rewritten to run parallel with multiple processors. In this study we will only report the data obtained from single-processor code.

6. Results and Discussions

The effect of solder microstructure coarsening on local stresses and strains was investigated using the code described above.

In 1-phase solder model, von mises stresses and strains vary gradually across the sample (refer to Figure 5) and they are symmetrical to center lines.. In reality, solder is a heterogeneous body consisting of two phases, Sn and Pb, and the stress and strain values and their distribution would be significantly different than that of 1-phase solder. The results for 2-phase microstructure, both lamellar and equiaxed, are described below.

Parametric Study of Lamellar Microstructure
Von Mises Stress & Strain Distribution: Figure 6 shows the distribution of von mises stresses in microstructure of different coarseness. The data shows that the Von mises stresses are higher within an order of magnitude of the yield strength values except at bottom right corner, where maximum stresses are seen. These observations confirms the results of many experimental studies, which have shown that thermal fatigue cracks initiate at the corners. In general, the stresses are higher in Sn phase. Figure 7 shows the distribution of von mises strains for varying grain coarseness. Again the strains are more heterogeneously distributed than observed in 1-phase solder (Figure 5). The strains are concentrated in Pb-phase.

Effect of Grain Coarsening on Stresses and Strains: The maximum stresses and strains increase with grain coarsening as seen in figures 6 & 7. Graphically, the maximum von mises Stress versus grain coarseness is shown in Figure 8. Stress values increase with grain coarseness. Also shown in this plot, the maximum stress value observed with 1-phase solder. 2-phase solder shows higher stress values for all grain coarseness investigated. As shown in Figure 7, there is a small increase in strain values with increasing coarseness. Moreover, the difference in strains between 2-phase (Figure 7) and 1-phase solder (Figure 5) is significantly higher.

Parametric Study of Equiaxed Microstructure
Distribution of stresses and strains: Stress distribution is shown in Figure 9. At fine coarseness, the stress variation is gradual. At higher coarseness, the stress distribution is more heterogeneous. The higher stresses are generally observed in Sn phase and the maximum stresses appear at the corners. Strain distribution is shown in Figure 10. The higher strains are concentrated in Pb phases and the higher strains are in the center and the corner of the domain.

Effect of Coarsening on Stresses and Strains: Figure 11 shows maximum von mises stress as a function of coarseness for two problem sizes, 36 and 72 elements per side. The data do not show any definite trend, increasing or decreasing, in the range shown. The equiaxed grains are generated with random numbers. It was observed that when the random number changes, the Sn and Pb phase distribution changes, giving a slightly different maximum stress and strain value.

The locations, where von mises stresses exceed yield stress, the material will plastically deform, and the plastic strains determine the fatigue behavior of solder. In this study, the yield stresses are exceeded and thus, more rigorous analysis using plastic model is needed. However, one can make qualitative statements about the relative degree of susceptibility to fatigue failures. Both lamellar and equiaxed microstructure show that von mises stresses exceed yield stresses and the maximum von mises stress is higher in 2-phase solder as compared to that in 1-phase solder. Thus 2-phase solder is likely to have higher plastic strains and thus it will be more susceptible to fatigue cracking.

Lamellar microstructure also shows gradual rise in von mises stresses with grain coarsening occurring during fatigue cycling. Thus lamellar microstructure will likely be more susceptible to fatigue failure. The computed results show that the von mises stresses in equiaxed microstructure are not significantly dependent on grain coarseness. Experimentally, investigators (ref 1) have found that fine, equiaxed microstructure has higher fatigue resistance than lamellar microstructure. This could be due to the fact that on the average, the strains and stresses do not increase with grain coarsening, and thus the fatigue life is not affected as in lamellar microstructure.

Since there is no direct experimental technique to obtain local stress and strain distribution within solder microstructure, this study has demonstrated the usefulness of parametric, virtual experiment. We have made some simplifying assumptions, but a more complex model can be easily built on this simpler model. A more rigorous approach, treating solders as non-linear, plastic material, with grain boundaries and intermetallics will be reported in the future.

7. Conclusions

An efficient code to study the effect of grain coarsening on the stresses and strains within computer-generated solder microstructure has been developed. The code involves (i) development computer –generated solder microstructures, lamellar and equiaxed, of varying grain coarseness, and (ii) finite element code. The FE code, specifically developed for this study, uses an algorithm involving the sparse matrix and iterative solver, which allows analysts to use over a million degrees of freedom.

In lamellar microstructure of 2-phase solder, von mises stresses and strains are heterogeneously distributed compared to the gradual variations seen with 1-phase solder. In general, the maximum stress and strain in 2-phase solder is higher than in 1-phase solder. The maximum von mises stress and strain in the lamellar microstructure gradually increases with grain coarseness.

In equiaxed microstructure of 2-phase solder, the stresses are heterogeneously distributed, but no general trend, increasing or decreasing, with coarseness was observed.

10. Acknowledgements

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References

1. "The Mechanics of Solder Alloys," Edited by D. Frear, H. Morgan, S. Burchett and J. Lau, Van Nostrand Reinhold, 1993.
2. "Soldering in Electronics," R. J. Klein Wassink, 2nd Edition, Electrochemical Publication Ltd, 1989.
3. "Handbook of Microelectronic Packaging" Edited by Rao Tummala and Eugene Rymaszewski, Van Nostrand Reinhold, 1989.
4. "Materials Handbook for hybrid microelectronics," Edited by Joseph Alison king, ARTECH HOUSE, Inc., 1988.
5. "Thermal Stress and Strain in Microelectronic Packaging," Edited by John Lau, Van Nostrand Reinhold, 1993.

Table 1: Material Properties

	Sn	Pb	1-Phase Solder
Young's Modulus(N/mm^2)	48625 (ref 2)	16000 (ref 2)	37500*
Poisson's Ratio	0.38 (ref 3)	0.38 (ref 3)	0.38*
Yield Stresses(N/mm^2)	6.9 (ref 4)	18** (ref 5)	10.6*

*Composite of 2 volumes of solder for every volume of Pb. **Assumed same as that of 95%Pb and 5% Sn.

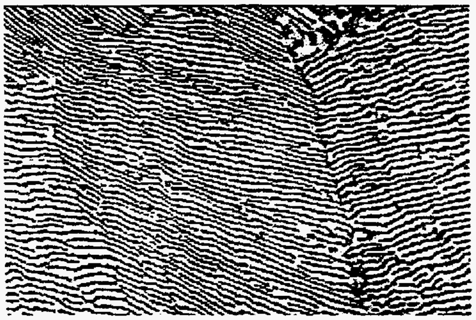

Figure 1: Lamellar microstructure obtained by slow cooling of eutectic solder (ref 1).

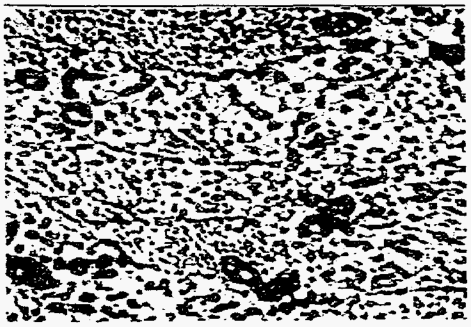

Figure 2: Equiaxed microstructure obtained by fast cooling of eutectic solder (ref 1).

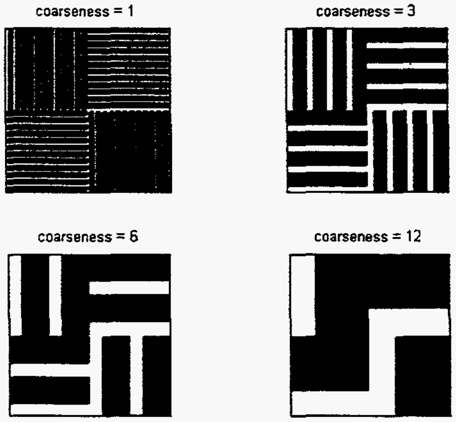

Figure 3: Computer-generated lamellar microstructures of varying grain coarseness (dark shade = Sn, white shade = Pb).

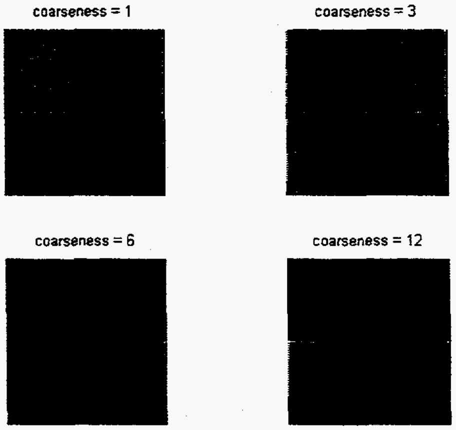

Figure 4: Computer-generated equiaxed microstructures of varying grain coarseness (dark shade = Sn, white shade = Pb).

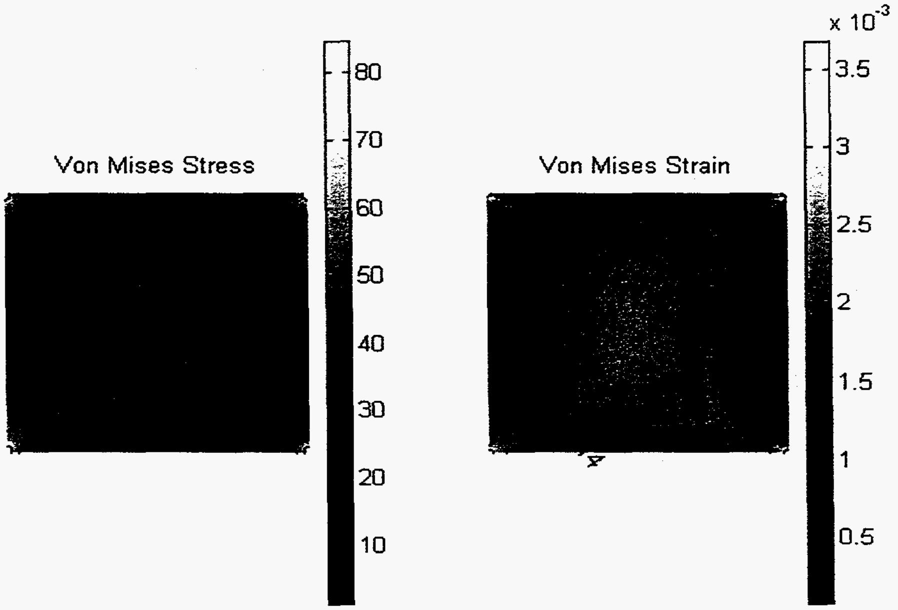

Figure 5: Von mises stress and strain distribution in 1-phase solder. All stress values are in N/mm^2 units.

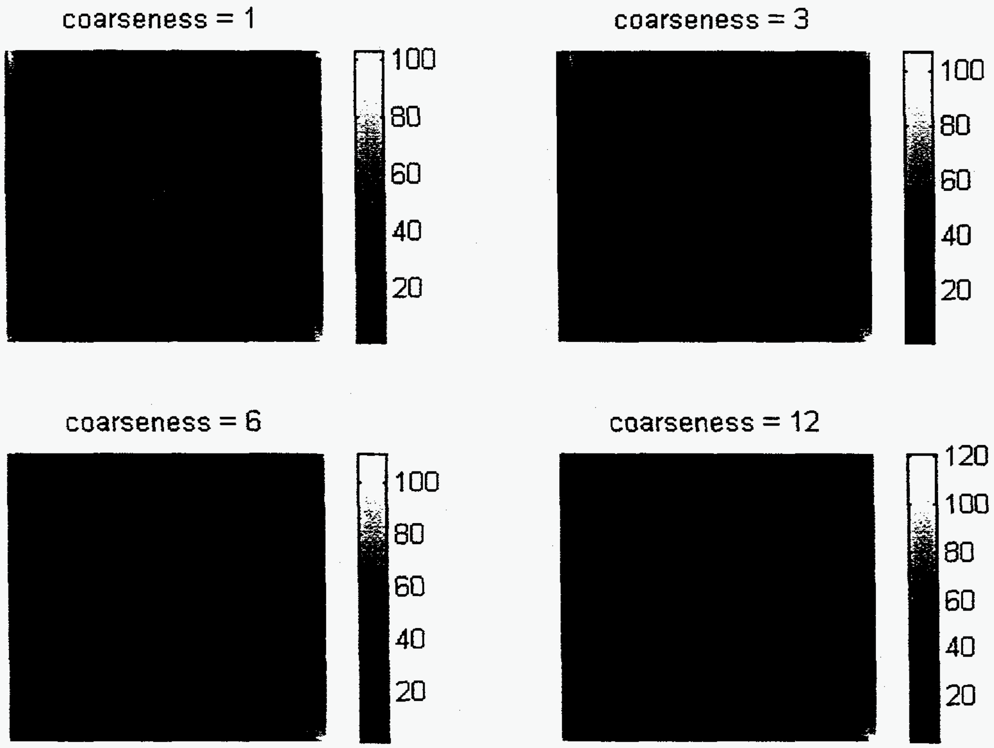

Figure 6: Von mises stress distribution for different grain coarseness in 2-phase, lamellar, solder microstructure (shown in Figure 3). All stress values are in N/mm^2 units.

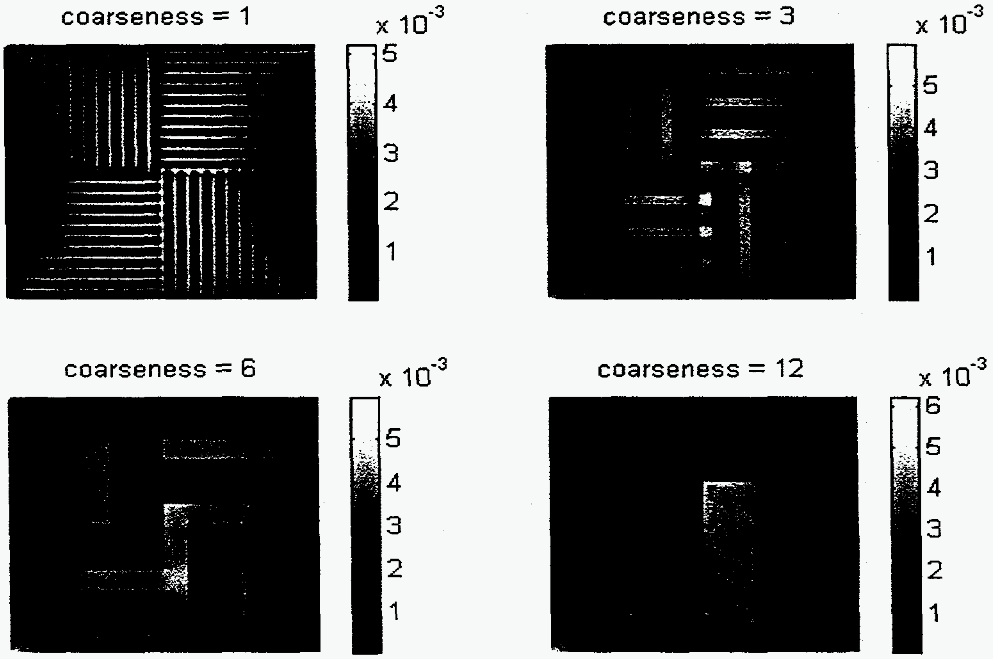

Figure 7: Von mises strain distribution for different grain coarseness in 2-phase, lamellar, solder microstructure (shown in Figure 3). All stress values are in N/mm^2 units.

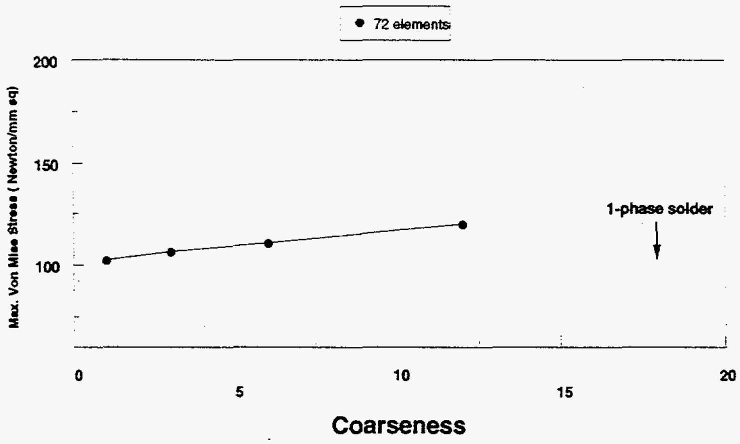

Figure 8: Max. von mises stress in solder microstructure as a function of grain coarseness for lamellar case.

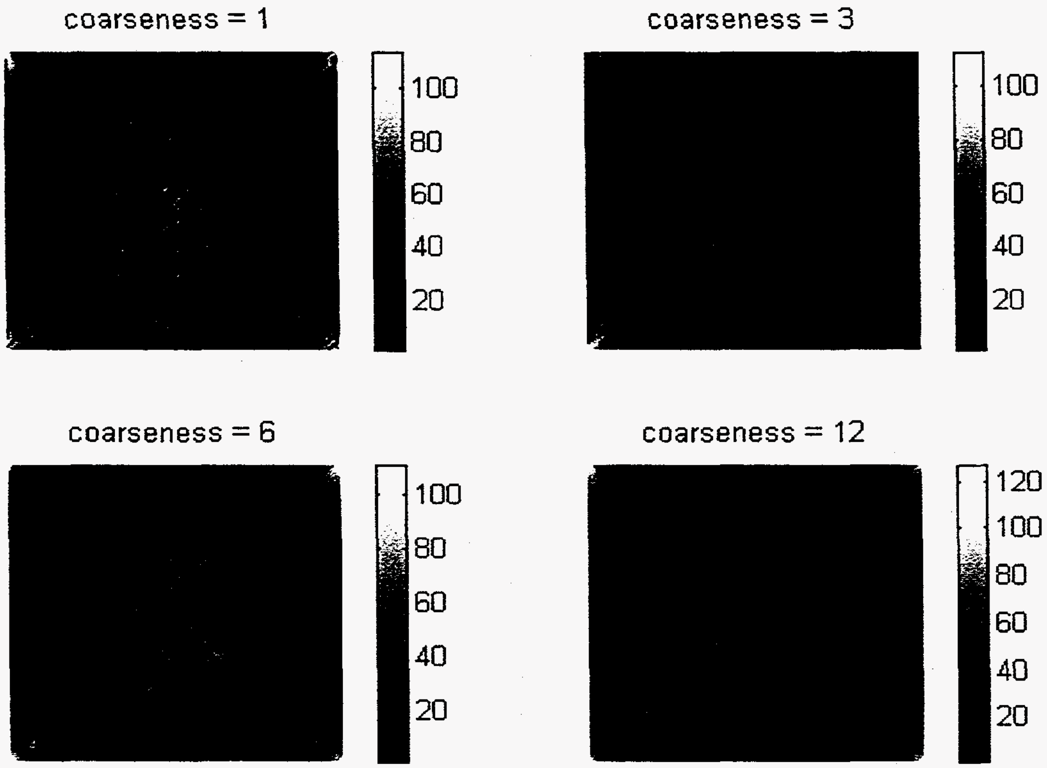

Figure 9: Von mises stress distribution for different grain coarseness in 2-phase, equiaxed, solder microstructure (shown in Figure 4). All stress values are in N/mm^2 units.

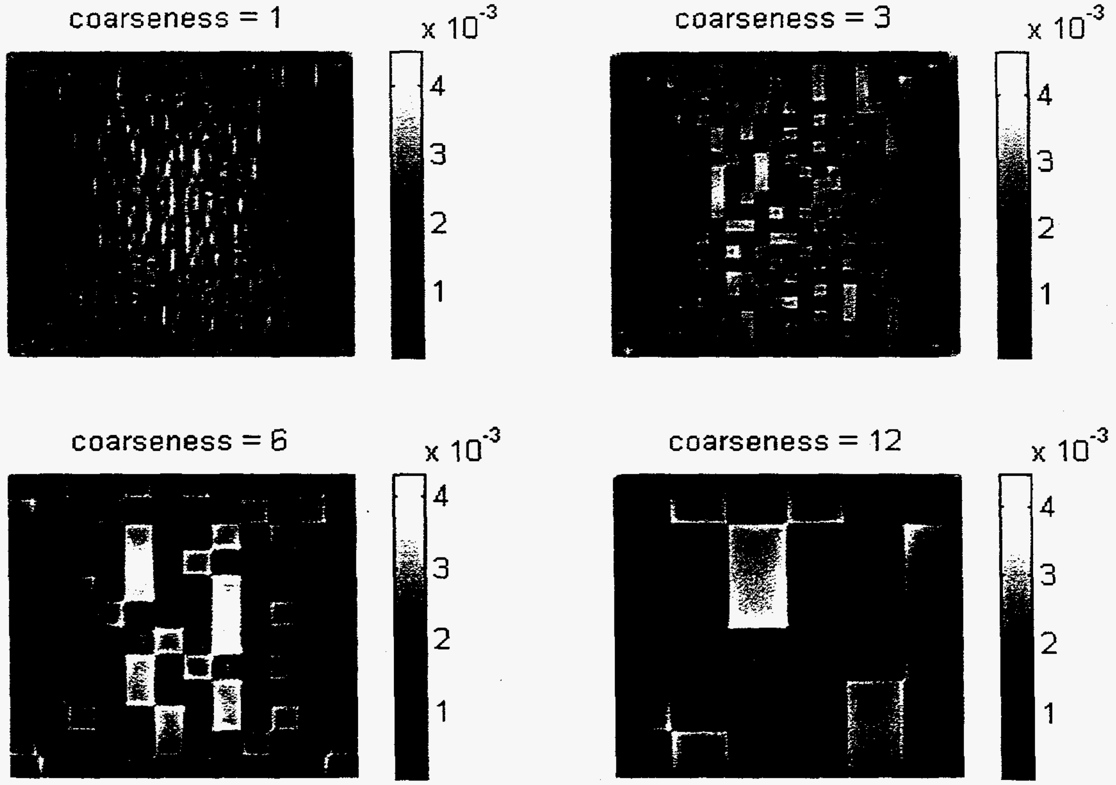

Figure 10: Von mises strain distribution for different grain coarseness in 2-phase, equiaxed, solder microstructure (shown in Figure 4). All stress values are in N/mm^2 units.

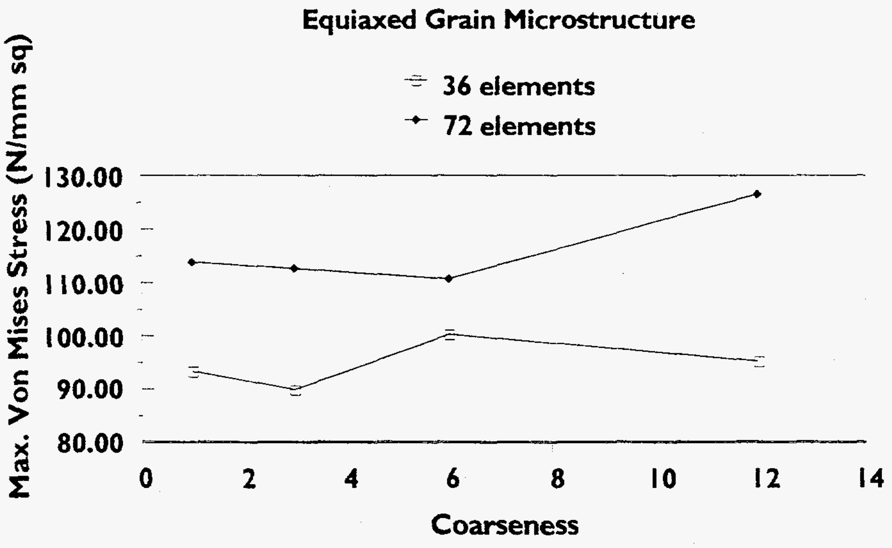

Figure 11: Maximum von mises stress in solder microstructure as a function of grain coarseness for equiaxed microstructure.