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Modelling the Deformation Behaviour of W/Cu Composites by a Self-Consistent Matricity Model

S. Schmauder, U. Weber, I. Hofinger, A. Neubrand

In the recent past, composites with interpenetrating microstructures of mechanically strongly different phases are of increasing importance as structural and functional materials in numerous industrial application fields. In order to design such composites, it is thus important to develop methods for predicting their thermo-elastic-plastic mechanical properties. In this paper, systematic analyses are presented for the W/Cu system with respect to modulus, thermal expansion coefficient, degree of interpenetration (matricity) and dependence of the plastic behaviour with respect to volume fraction, matricity and thermal expansion mismatch of the phases. Besides these global parameters the frequency distributions of total strains as a measure of deformation in the phases is obtained.

1 Introduction

Composites consisting of phases with strongly different properties have the potential to be used in new application fields as they comprise otherwise incompatible properties. While the deformation behaviour of inclusion-type of microstructures has been successfully modelled in the past for brittle fiber or particulate reinforced metal matrix composites (Zahl et al., 1994; Dong and Schmauder, 1996a) this was not achieved until recently in the case of interpenetrating microstructures where both phases are connected throughout the material. Such microstructures are typically observed in the composition range of 30÷70% while inclusion type of microstructures are typical for dilute systems with phase volume fractions between 0÷30%. Specifically, functionally graded materials can depict the full composition range in material transitions. As processing techniques are nowadays available to design material transitions, experience in modelling of the full composition range is still lacking. This paper is intended to bridge this gap in the case of W/Cu composites where the full compositional range is available from a powder-metallurgical route (Jedamzik et al., 1997), such that comparison in properties and predictions can be made.

2 Models

Three models are used for the simulation of the thermo-elastic-plastic materials properties of composites with phases α and β in this paper. In the case of an inclusion type of microstructure the self-consistent embedded cell model is applied which is described in (1., 2., 12., 13., 19.). The embedded cell model has been introduced to simulate the mechanical behaviour of composites with randomly distributed inclusions. The volume fraction of the inclusions is the main parameter in the model. To take the matricity as a second microstructural parameter into account, the self-consistent embedded cell model has been extended by a second self consistent embedded cell model (Figure 1). In this "matricity model" we are able to define the matricity of the model in the same manner as the matricity is defined for a real microstructure: First the single phases are reduced to skeleton lines. The lengths of the skeleton lines of the inclusions (Figure 1; left:β, right:α) are zero as the inclusions are spherical and are, therefore, reduced to a point in the process of obtaining the matricity of the phase.
The lengths of the skeleton lines S_α and S_β in the matrices are given as the circumference of a circle with a diameter which is obtained from the arithmetic average of the diameter of the embedded cell and the diameter of the inclusion phase (Figure 1; left: S_α, right: S_β). The diameters of the embedded cells are denominated as W_1 and W_2. The diameters of the inclusion part of the embedded cells depend on the volume fraction of the inclusions and the corresponding factors W_1 or W_2. The matricity M can be calculated as a function of the sizes of the embedded cells and the volume fraction of one of the two phases, as the volume fraction of the phases is held constant in both parts of the matricity model.
As can be seen in Figure 1, the volume fractions of the phases as well as the diameters W_1 and W_2 of the embedded cells are adjustable. To achieve a matricity M_i ($i=\alpha, \beta$) in the model, the measured volume fraction of the phases in the model is realized and the diameters W_1 and W_2 are calculated according to equation 1 (Leßle et

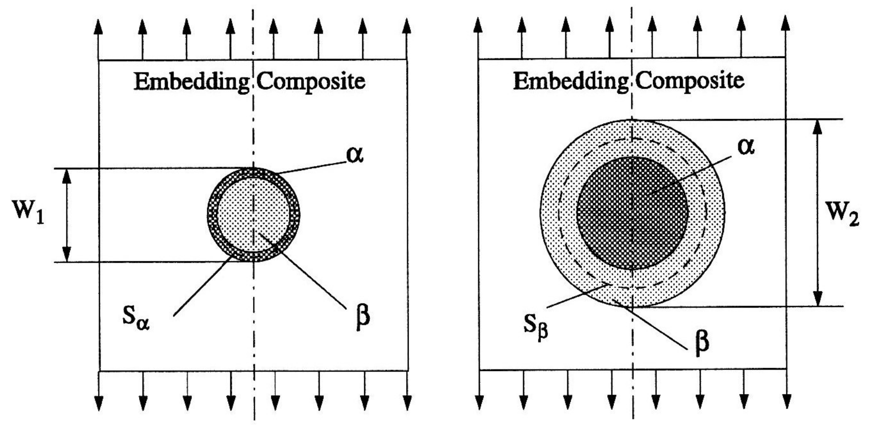

Figure 1. Matricity-model (schematic) with Skeleton Lines to Adjust for the Measured Parameter „Matricity“ in the Model via the Factors W_1 and W_2.

$$W_1 = W_2\left(\sqrt[3]{1-f_\beta}+1\right) \cdot \frac{1-M_\beta}{M_\beta\left(\sqrt[3]{f_\beta}+1\right)}, \quad W_2 = 1 \text{ for } M_\beta \geq 0{,}5$$

$$W_2 = W_1\left(\sqrt[3]{1-f_\alpha}+1\right) \cdot \frac{1-M_\alpha}{M_\alpha\left(\sqrt[3]{f_\alpha}+1\right)}, \quad W_1 = 1 \text{ for } M_\alpha \geq 0{,}5 \qquad (1)$$

al., 1998). If the geometrical boundary conditions are modelled at a distance of about 5 times the radius of the embedded cell, they are of almost no influence on the model's mechanical behaviour. If the boundary conditions are kept remote the embedded cell can be modelled with the surrounding composite in different manners. As the remote boundary conditions have almost no influence on the mechanical behaviour of the embedded cell it is assumed that the continuum mechanical stress-strain state in the embedded cell is hardly influenced as well. Taking this into account, a unit cell for a specific volume fraction can be used in each part of the matricity model. Moreover, due to the virtual independency from remote boundaries, it is not necessary to model the matricity as an absolute parameter of the FE-mesh. It is rather possible to introduce the matricity by adjusting weighting factors W_1 and W_2 only in the evaluation of the results from the inclusion type geometries. As the results have to be determined by an iterative procedure in about 3 to 5 iterations, the adjusting weighting factors W_1 and W_2 must be introduced in the evaluation of each iteration step.

In principle, stress-strain curves of the two-phase composite are determined from the matricity model in the same iterative manner as it is done for the simple self-consistent embedded cell model: In each increment the components for stress and strain are determined. This is done by a weighted averaging of the stress and strain values over all integration points of both embedded cells.

Interpenetrating microstructures where both phases can show percolation throughout the material are characterized by the above introduced matricity parameter M with values between 0 and 1 describing the mutual material circumscription of the phases in addition to their volume fractions. The matricity model is based on a numerical scheme consisting of inclusions of a given volume fraction and with circular cross-section (3., 7., 9., 10., 14.-16., 20.). The model in Figure 1 allows for the consideration of thermal residual stresses and can be used to predict the elastic properties, the thermal expansion coefficient and the elastic-plastic stress-strain curves for the different phase arrangements as well as to predict phase properties of the phases in the composite. For comparison reasons the Tuchinskii model is introduced as second model which allows to predict upper and lower bounds of the elastic modulus of a composite with interpenetrating microstructures by the following formulae (Tuchinskii, 1983) where E_i = Young's modulus of phase i, f_i = volume fraction of phase i (i=A, B; C=composite).

$$\frac{E_C}{E_A} = (1-c)^2 + \left(\frac{E_B}{E_A}\right)c^2 + \frac{2(E_B/E_A)c(1-c)}{c+(E_B/E_A)(1-c)} \qquad \text{lower bound} \qquad (2)$$

$$\frac{E_C}{E_A} = \left[\frac{1-c}{(1-c^2)+(E_B/E_A)c^2} + \frac{c}{(1-c)^2+(E_B/E_A)(2-c)c}\right]^{-1} \qquad \text{upper bound} \qquad (3)$$

$$f_B = (3-2c)\cdot c^2 \qquad \text{relation between volume fraction and geometric parameter c} \qquad (4)$$

In a third model by Pompe the calculation of the thermo-elastic constants is also based on the solution of an inclusion problem (Kreher and Pompe, 1989). Due to their ellipsoidal shape the fields inside the inclusions are homogeneous and can be determined analytically. Throughout this paper we assume the special case of spherical inclusions. Interaction between the media can be considered through assumptions about the surrounding material. This is often realized by the effective medium theory (EMA). For the mean stress and strain fields self-consistency must be claimed leading to an implicit equation system which allows for determination of the effective constants. The effective values for Young's modulus and thermal expansion coefficient have been determined numerically.

3 Results and Discussion

W/Cu compositions in the range of 3÷75% Cu were produced by a sintering and infiltration method (Jedamzik et al., 1997). The corresponding microstructures are presented in Figure 2. Besides the volume fraction, a second parameter, the so-called matricity parameter M which represents the degree of mutual interpenetration and

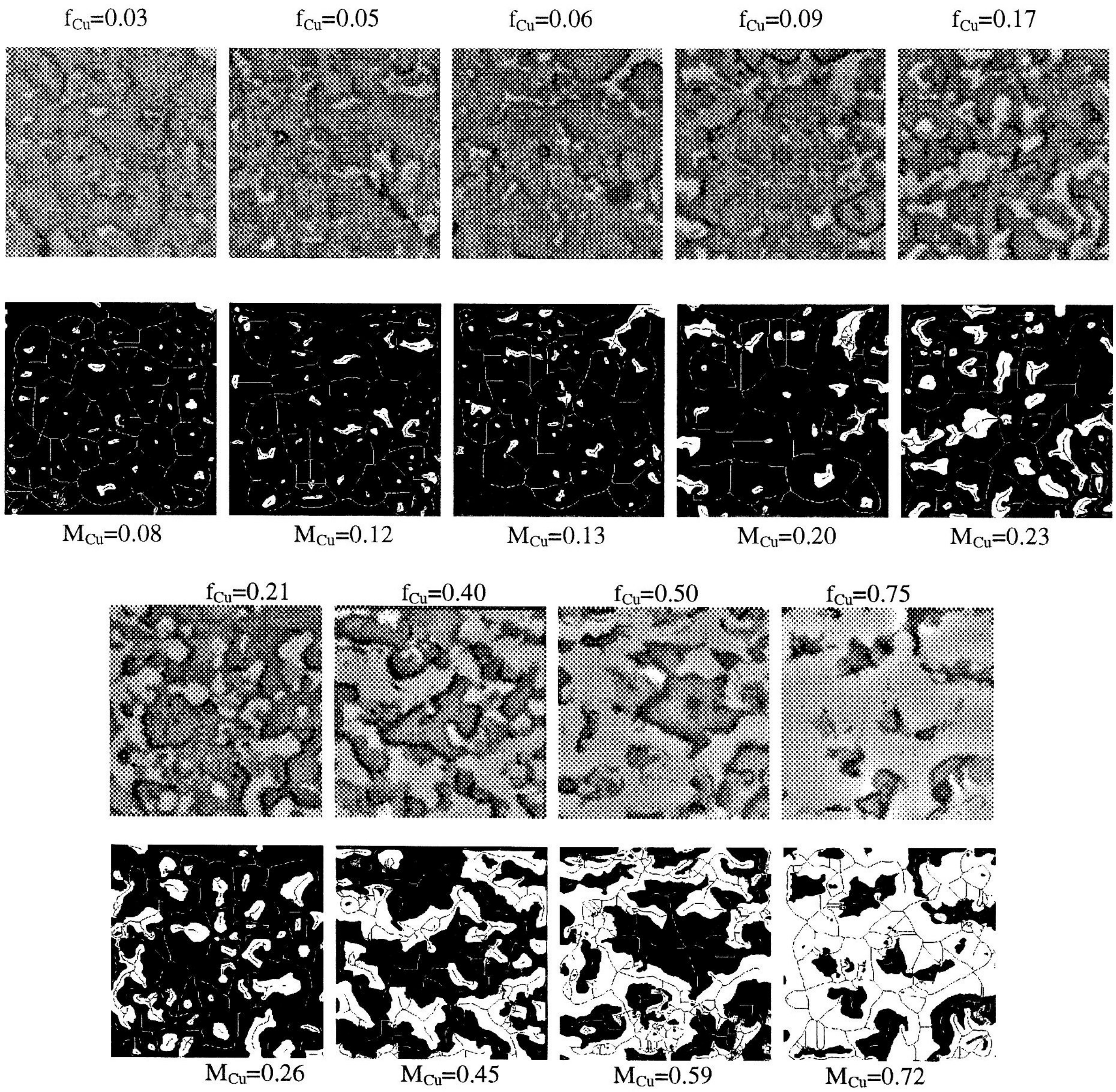

Figure 2. Microstructures and Matricities of Different W/Cu Composites.

circumvention of the phases and which was introduced by (Poech and Ruhr, 1993) is also given in the figure. In the following, composites of two phases α and β are considered. Matricity is then defined as the fraction of the length of the skeleton lines of one phase, S_α, and the length of the skeleton lines of the participating phases

$$M_\alpha = S_\alpha / (S_\alpha + S_\beta) \tag{5}$$

By definition, the sum of the matricities of all phases equals one

$$M_\alpha + M_\beta = 1 \tag{6}$$

To obtain the skeleton lines of a certain phase, this phase is selected within an image analysing system and the detected structure is reduced to a typically non-connecting line maintaining the topology. In Figure 2 the matricities have been determined for a graded W/Cu composite. The structure parameters, volume fraction f, and matricity M, have been determined to be, e.g., M_{Cu}=0.08, 0.26, 0.45 and 0.72 for f_{Cu}=0.03, 0.21, 0.40 and 0.75, respectively. It can be seen that although there exists a nearly linear relationship between the two parameters (Figure 3) the slope is clearly less than 0.9. M is linearly related to the cluster parameter r_α: $M = a{\cdot}r_\alpha + b$, a=0.4, b=0.3 (Appendix).

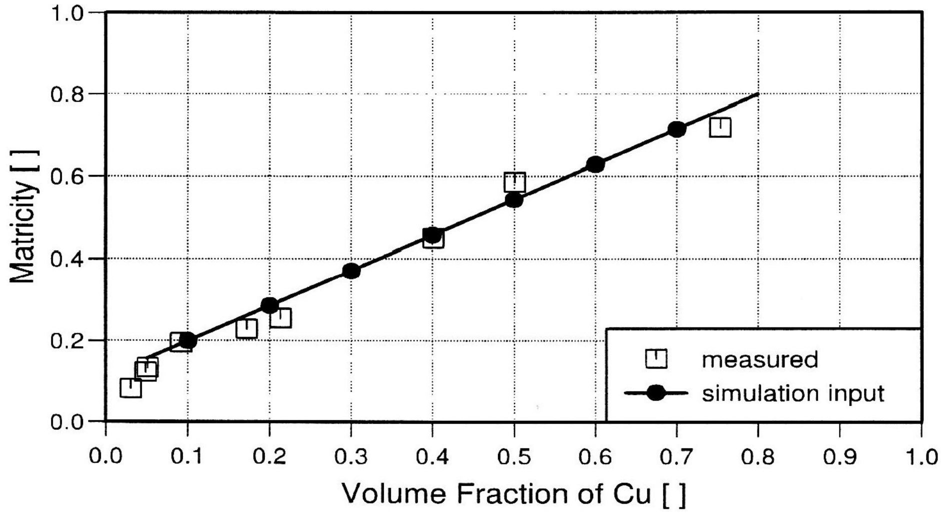

Figure 3. Correlation between Volume Fraction and Matricity for Different W/Cu Microstructures.

The experimental data of Young's modulus were determined using a resonance method according to ASTM C1259-94. For this purpose quasi-homogeneous rectangular bars of 0.4 mm thickness t, 4 mm width b and 22 mm length L were cut from the W/Cu sample using a wire saw. A piezoelectric transducer was attached to one

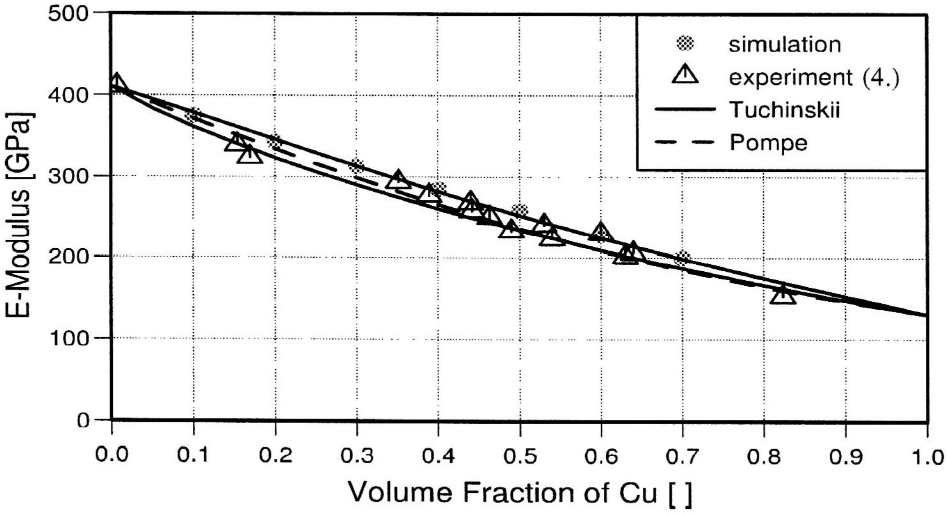

Figure 4. E-Modulus for the Different W/Cu Microstructures.

end of the bars and a magnetic pickup to the other end with a thin thread. The frequency F of the fundamental flexure mode of the bars was determined by a computer-controlled frequency generator/lock-in amplifier combination. The dynamic Young's modulus E of each region was then calculated from the mass m and the dimensions of the bars according to ASTM Designation C 1259-94 (21.)

$$E = 0.9465 \cdot (m \cdot F^2 / b)(L^3 / t^3)(1 + 6.585 \cdot t^2 / L^2) \tag{7}$$

The elastic behaviour of the composite is represented in Figure 4 where the Young's modulus is seen to vary between those of the components at f=0 and f=100%. It is interesting to see that the predictions of the upper and lower bounds from the Tuchinskii model are rather close to each other, while the moduli of W and Cu differ by a factor of 3.16. The experimental values fall into these bounds and the matricity model predictions are in the same range. The experimental data are very well described by the Pompe model. The thermal expansion coefficient of the composite as observed in the experiments obeys the rule of mixture (between α_W=4.7E-6·1/K and α_{Cu}=18.9E-06·1/K) in good approximation and so does the calculation when thermal stresses are taken into account (Figure 5). The agreement between the simulation and the Pompe model is very good. Earlier results on metal/ceramic composites have shown that the thermal expansion coefficient α is nearly independent on M (Leßle, 1997).

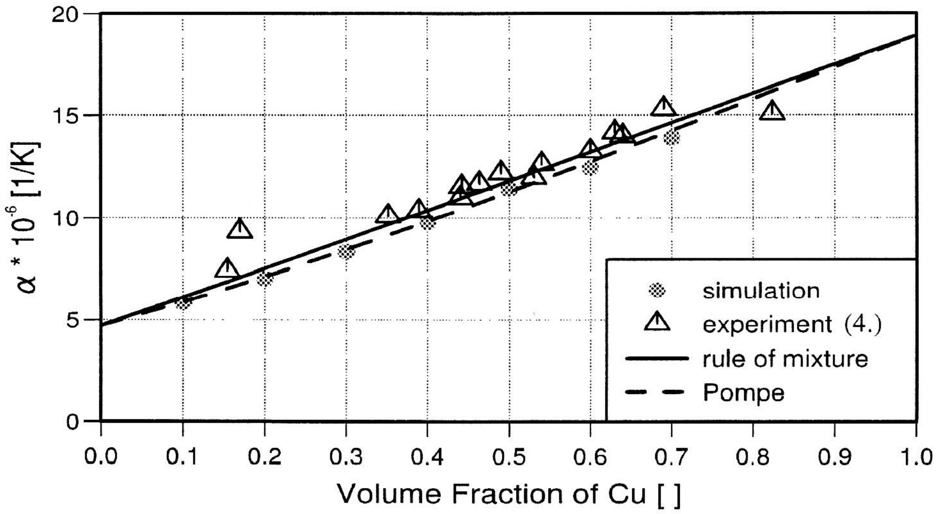

Figure 5. Thermal Expansion Coefficients of the W/Cu Microstructures.

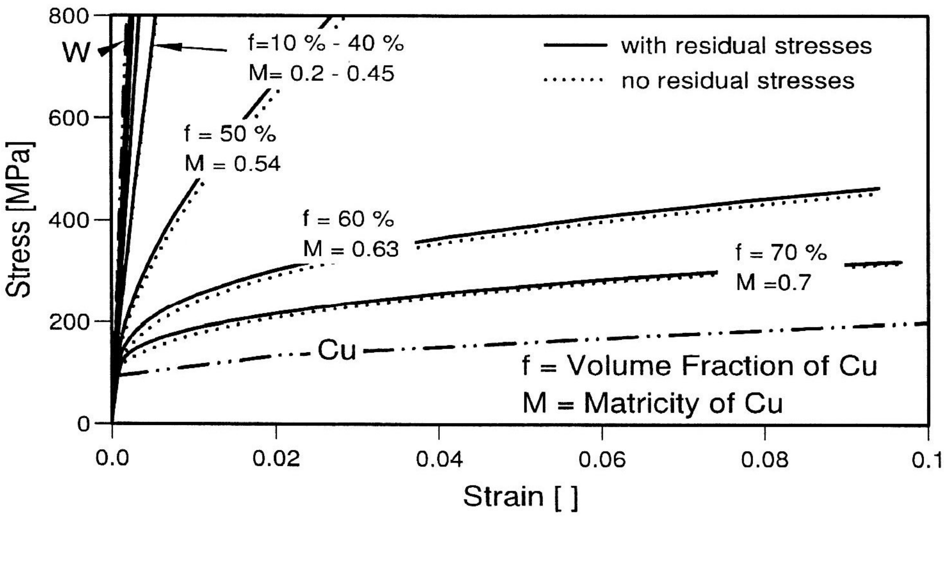

Figure 6. Calculated Stress-strain Curves and Influence of Thermal Stresses for Selected Compositions and According Matricities for the Different W/Cu Microstructures.

The model predictions for the stress-strain curves of W/Cu (with the corresponding volume fractions and matricities of the real composites) are depicted in Figure 6, where a strong variation in the mechanical behaviour is seen for $f_{Cu} = 0.4 \div 0.7$. The influence of residual stresses caused by cooling down the material from processing to environmental temperature is also indicated in this figure. Obviously, no strong influence of the residual stresses is observed. Nevertheless, the residual stress distribution can be predicted reliably in either phase, as shown in (Leßle et al., 1998). Decoupling of the parameters (f_{Cu}=50%, M=variable) demonstrates that phase arrangement is the parameter which actually controls the mechanical behaviour of the W/Cu composite (Figure 7).

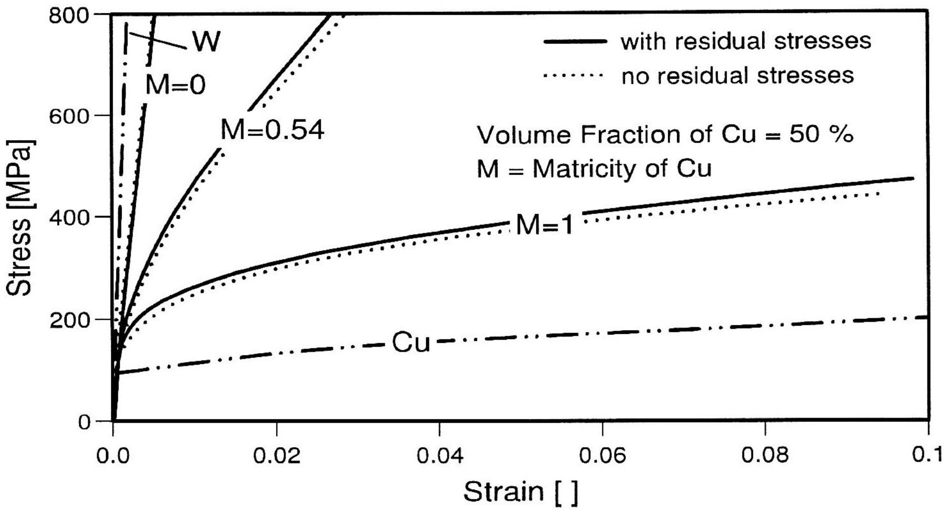

Figure 7. Calculated Influence of Matricity and Residual Stresses for W/Cu Composites.

Another interesting parameter to analyse is the frequency distribution of the strains in either phase (Figure 8 and Figure 9) at a given global strain of, e.g., 5 % of the composite (with f_{Cu}=60 %, M_{Cu}=0.64). Two main features can be seen: First, the Cu phase carries most of the strain with an average value of ~ 7 % which is well above the composite strain. And second, the strain values are widely distributed in the Cu phase (-1% ÷ 19%) compared to the W phase (average: 0,13%, range: 0.07÷0.225%). This aspect is important with respect to considerations of crack nucleation in the phases.

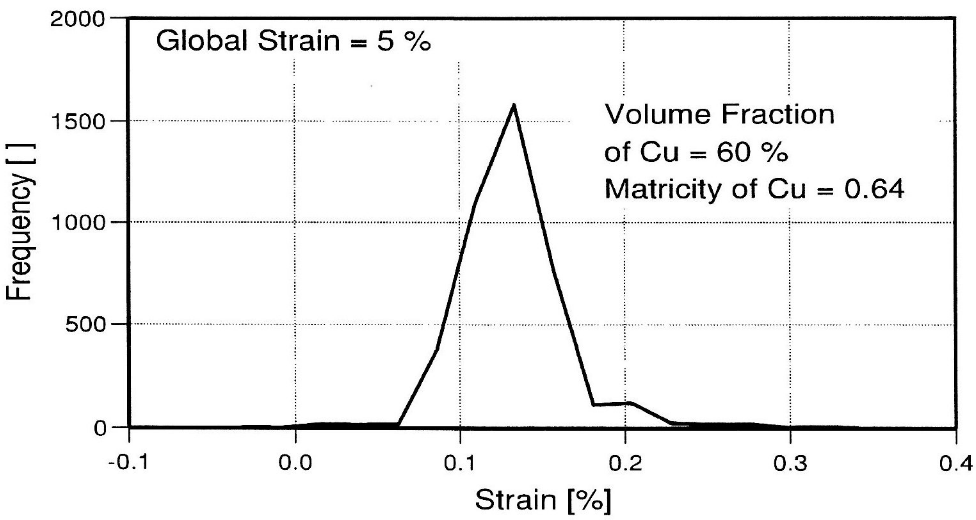

Figure 8. Frequency Distribution of Total Strains in W Phase in W/Cu Composites at a Global Strain of 5% (f_{Cu} = 60% and M_{Cu} = 0.64).

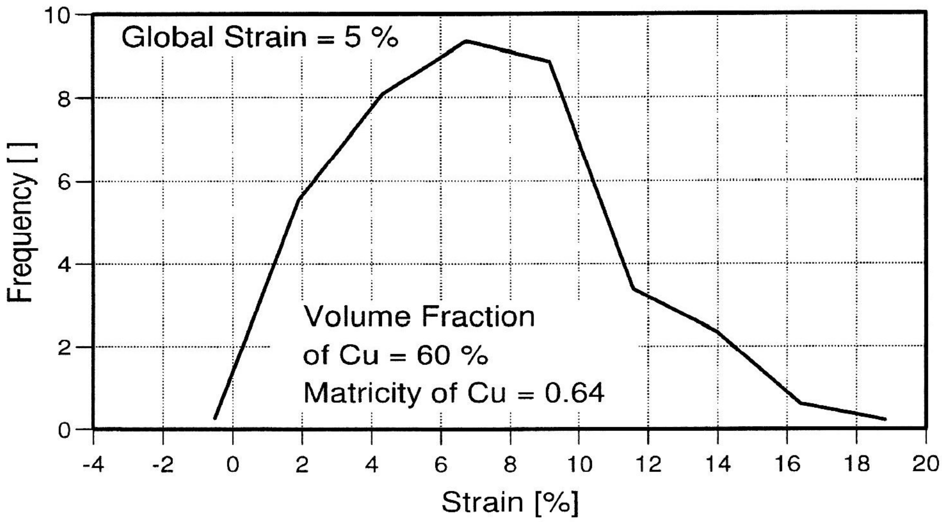

Figure 9. Frequency Distribution of Total Strains in Cu Phase in W/Cu Composites at a Global Strain of 5% (f_{Cu} = 60% and M_{Cu} = 0.64).

4 Conclusions

The matricity model was applied to systematically predict the thermo-elastic-plastic material properties of a full range of W/Cu compositions. Comparisons were made with experimental results on the thermo-elastic-plastic properties and with the Tuchinskii model and Pompe model for elastic properties. The results in the case of W/Cu (with one elastic and one elastic-plastic phase) can be summerized as follows:

- The expansion coefficient of the composite is not dependent on the matricity parameter and thus well predicted by the linear rule of mixture. Residual stresses do have a minor influence on α.
- The elastic modulus is well predicted by the Tuchinskii model as well as by the matricity model and by the Pompe model.
- The stress-strain curve is strongly influenced by volume fraction (in the range of f_{Cu} = 30-70%) and by the matricity parameter M. Again, small effects were found from residual stresses.
- While the W phase carries most of the stresses, the frequency distribution of total strains demonstrates that the softer phase is strained to a level higher than the composite in average.

Appendix

Recently, Siegmund et al. introduced the so-called cluster parameter r_α which gives the relative number of clusters NC(α) of phase α in phase β in an α-β-composite r_α=NC(α)/(NC(α)+NC(β)). In [Siegmund et al., 1993] this parameter was calculated for a number of artificial microstructures consisting of equally sized hexagons. More recently, [Leßle et al., 1996] have measured the matricity parameter for the same microstructures. It was found that M and r_α are linearly correlated. The superiority of M versus r_α is due to a wide range and a simpler determination of the matricity value [Leßle et al., 1996].

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Addresses: Prof. Siegfried Schmauder and Dipl.-Ing. Ulrich Weber, Staatliche Materialprüfungsanstalt (MPA), University of Stuttgart, D-70569 Stuttgart, Dr.-Ing. Ines Hofinger, University of Dresden, D-01062 Dresden, Dr. Achim Neubrand, University of Darmstadt, D-64287 Darmstadt