MICROMODELLING OF CREEP IN COMPOSITES WITH PERFECT MATRIX/PARTICLE INTERFACES

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A new micromechanical model of creep in composites with perfect matrix/particle interfaces is suggested. The model assumes that particles are harder than the matrix and the plastic deformation in the matrix is due to time-dependent slip in discrete slip systems. Slip in the matrix causes the deposition of dislocations on the matrix/particle interfaces hindering further slip. Creep in the composite is conditioned by dynamic recovery due to the slip/climb motion of the dislocations along the matrix/particle interface to places where the dislocation loops disappear. The mentioned processes are described by proper equations. The equations are solved by finite element method (FEM) and a special FEM code is used for the micromodelling of creep in superalloy single crystals.

MIKROMODELOVÁNÍ CREEPU V KOMPOZITNÍCH MATERIÁLECH S DOKONALÝM ROZHRANÍM MEZI MATRICÍ A ČÁSTICEMI

Je navržen nový mikromechanický model creepu v kompozitních materiálech s dokonalým rozhraním mezi matricí a částicemi. Model předpokládá, že částice jsou tužší než matrice a plastická deformace matrice vzniká časově závislým skluzem v diskrétních skluzových systémech. Skluz v matrici způsobuje hromadění dislokací na rozhraní mezi matricí a částicemi bránící dalšímu skluzu. Creep v kompozitním materiálu je podmíněn dynamickým zotavením způsobeným nekonzervativním pohybem dislokací podél rozhraní mezi matricí a částicemi na místa, kde dislokační smyčky mizejí. Zmíněné procesy jsou popsány odpovídajícími rovnicemi. Rovnice jsou řešeny metodou konečných prvků; pro mikromodelování creepu monokrystalů superslitin je použit speciální program vycházející z této metody.

1. Introduction

The most effective way how the creep resistance of metals can be improved is their reinforcement by hard particles. The particles can precipitate in the matrix

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during the heat treatment of the material as in the case of superalloys. The particles can also be added into the matrix or they precipitate in the matrix during solidification as, e.g., in case of metal-matrix composites.

The creep resistance of composites depends critically on the properties of the interfaces between the matrix and particles. In case of practically non-wetting particles the matrix/particle decohesion can easily occur during creep [1] and the creep properties of the composite are worse than those of the matrix. The non-coherent interface with good wetting properties is the next type of the interface. Such interface can act as a channel of high diffusivity and a place of easy sliding analogous to grain boundary sliding. Moreover the interface can act as a source and sink of vacancies and it can also absorb dislocations. The creep properties of such composites have been studied in [2]. In the paper it was shown that the creep resistance of the composite can be significantly influenced by the properties of the matrix/particle interface which is in accord with the earlier work of Goto and McLean [3]. The interfaces with low diffusivity and low capability of sliding imply the best creep properties of the composite. The interfaces with practically zero diffusivity and zero capability of sliding are realized either as coherent interfaces (semicoherent if misfit dislocations are deposited on the interface) or as interfaces of the type Al/Al_2O_3. In the case of Al/Al_2O_3 interface, there is a strong reaction between the atoms of both phases and they form a perfect contact although their lattices and their lattice orientations are different. From the phenomenological point of view the coherent interfaces and interfaces of the Al/Al_2O_3 type can be treated as perfect interfaces with zero diffusivity and zero capability of sliding. They cannot act as sources and sinks of vacancies and of dislocations. Such interfaces represent usually an effective barrier for dislocations in the matrix. If there are no sources of dislocations in the particles, the particles behave like hard particles which is the case of superalloys. In case of metal matrix composites the ceramic particles are also much harder than the matrix.

The problem of creep in composites with perfect interfaces has been modelled by FEM in [4] (metal matrix composites) and in [5, 6] (superalloy single crystals). The authors treat the creep in the matrix as non-linear viscoplasticity. The properties of the matrix are assumed to be isotropic and except the exponent in the power law the matrix behaves like a very viscous fluid. During creep in the composite significant pressure gradients are developed in the matrix. In the proximity of the particle the matrix shears along the interface although in reality such slip systems need not be available.

If the particles are harder than the matrix, the composite under creep conditions deforms by slip in the matrix and the dislocations remain deposited on the matrix/particle interface or in its vicinity. The deposited dislocations cause a back-stress which hinders further plastic deformation in the matrix. Thus, creep of the composite is conditioned by dynamic recovery of the dislocation structure.

If the dislocations cannot cut the particle, the only possible recovery mechanism is climb/slip motion of dislocation loops along the matrix/particle interface to places, where the loops can shrink and disappear [7, 8]. This motion of dislocation loops is connected with the transport of atoms which are collected and deposited at jogs on moving dislocation loops. The transport of atoms represents diffusional creep controlled by lattice diffusion in the matrix. On the other hand, the diffusional creep is conditioned by the existence of dislocations with jogs acting as only sources or sinks of atoms on the matrix/particle interface.

It is obvious that the description of creep in the matrix by non-linear viscoplasticity represents only a rough approximation of reality. The main aim of the present paper is to incorporate the processes described in the previous paragraph into the FEM code. To reach this aim it is necessary:

(i) to apply the equations for the time-dependent crystal plasticity in the matrix,

(ii) to derive the equations for the rate of deposition of dislocations from each slip system at each point of the matrix/particle interface due to crystal plasticity,

(iii) to develop the model of recovery due to climb/slip motion of dislocations along the matrix/particle interface involving the changes of the dislocation density at each point of the interface,

(iv) to develop the mathematical method coupling the problems of elasticity and of (i)–(iii).

The code is applied to the modelling of creep in superalloys.

2. Physical background

2.1 Slip rate in the matrix

First approach on crystallographic modelling of creep in superalloys was presented by Ghosh et al. [9, 10]. The authors did not reflect the two-phase structure of the superalloys and recovery. Creep of the superalloy was treated as a cooperation of crystallographic slip and damage.

We assume that there are N slip systems in the matrix given by the unit normals to the slip plane $\boldsymbol{c}^k = (c_1^k, c_2^k, c_3^k)$ and by the unit vectors of slip directions $\boldsymbol{a}^k = (a_1^k, a_2^k, a_3^k)$, $k = 1, \ldots, N$. The resolved shear stress τ^k in the slip system is

$$\tau^k = \sum_{i,j=1}^{3} \sigma_{ij} a_i^k c_j^k, \tag{1}$$

where $\underline{\sigma}$ is the local stress tensor. The force per unit length driving the dislocation slip is given by

$$f^k = \beta(\tau^k - \frac{\gamma \kappa^k}{\beta}), \tag{2}$$

where β is the magnitude of the Burgers vector $\beta \boldsymbol{a}^k$, γ is the energy of dislocation per unit length and κ^k is the curvature of the dislocation line. For the energy of dislocation per unit length the expression

$$\gamma = \frac{1}{2} G \beta^2 \tag{3}$$

is usually used where G is the elastic shear modulus. The term $\gamma \kappa^k / \beta$ is called Orowan stress, τ^k_{Orowan}, and it is extremely important in systems where the matrix between particles forms very thin layers like in superalloys. In this case the curvature of the leading dislocation segment, the motion of which causes plastic deformation of the matrix, is very high. If h is the thickness of the matrix channel oriented in $\langle 001 \rangle$ direction and $\{111\}$ are the slip planes, then

$$\kappa^k = \frac{2\sqrt{2}}{\sqrt{3}h} \tag{4}$$

and the Orowan stress is then

$$\tau^k_{\text{Orowan}} = \sqrt{\frac{2}{3}} \frac{G\beta}{h} . \tag{5}$$

The velocity of the leading dislocation segment can be assumed to be in the first approximation proportional to the term $(\tau^k - \tau^k_{\text{Orowan}})^n$, where $n \geq 1$ is the stress exponent. Further we assume that the density of the leading dislocation segments is constant and thus the creep rate in the matrix is proportional to the term $(\tau^k - \tau^k_{\text{Orowan}})^n$. This assumption is not fulfilled in the very early stage of creep in superalloy single crystals which exhibit the incubation period. The virgin single crystal is nearly dislocation free and the mobile dislocations must first multiply by slip. Such effects are not studied in this paper.

In the frame of the small-strain approximation the creep rate (the "dot" symbol is reserved for the time derivative) of the matrix corresponding to the k^{th} slip system can be expressed as

$$\dot{\varepsilon}^k_{ij} = A(\tau^k - \tau^k_{\text{Orowan}})^n_+ b^k_{ij} , \tag{6}$$

where A is a proportionality constant, $(\ldots)_+$ denotes the positive part of $(\ldots)$ in sense

$$(\ldots)_+ = \begin{cases} (\ldots) & \text{for } (\ldots) > 0 , \\ 0 & \text{otherwise} , \end{cases} \tag{7}$$

and for the simplicity

$$b^k_{ij} = \frac{1}{2}(a^k_i c^k_j + a^k_j c^k_i) . \tag{8}$$

2.2 Deposition of dislocations

In materials with low fraction of reinforcing particles, the dislocations form usually the subgrain structure inside grains during creep. The subgrain boundaries are not fixed and the subgrain size depends on the history of the specimen.

In our treatment of composite materials, we suppose that the matrix forms a fine skeleton of the thickness much lower than the typical subgrain size. In superalloys the thickness of matrix channels is about 0.05 μm, while the typical subgrain size in crept materials is about 1 μm. The fact that the thickness of the matrix skeleton is lower than the typical subgrain size has the following consequences:

- The creep properties of the matrix can be completely different from those of the matrix material on its own.
- No subgrain structure will be formed in the matrix.
- The rate of generation of dislocations in the composite is determined by gradients of the slip rate in the individual slip systems. If the matrix/particle interfaces are effective barriers for the dislocation slip, the matrix/particle interfaces are the places of extremely high gradients of the slip rate and thus the places of deposition of dislocations.

During creep in the composite the dislocations are produced by slip in the matrix and annihilated by recovery. In the model we assume that the dislocations are localized only on the matrix/particle interface. This assumption is later confirmed by computation of creep in superalloys.

The dislocations deposited on the matrix/particle interface are the mixture of dislocations corresponding to the various slip systems. The dislocations corresponding to the k^{th} slip system are characterized by the Burgers vector $\beta \boldsymbol{a}^k$, by the dislocation line which is the section of the slip plane and the matrix/particle interface and by the dislocation density ρ^k (in units m/m^2; $1/\rho$ is the distance between dislocations). As $\beta \boldsymbol{a}^k$, $\boldsymbol{c}^k$ and the matrix/particle interface are assumed to be fixed in the frame of the small-strain approximation, the local densities ρ^k are parameters which describe unambiguously the actual dislocation structure. Assuming no slip in the particle, the rate of generation of dislocations $\dot{\rho}^{k+}$ must be proportional to the slip rate of the matrix in the k^{th} slip system in the vicinity of the interface. Analogously as in [11], it can be derived (see Appendix) that

$$\dot{\rho}^{k+} = \frac{A}{\beta} \sqrt{1 - (\boldsymbol{c}^k \cdot \boldsymbol{n})^2} \cdot (\tau^k - \tau^k_{\text{Orowan}})^n_+ , \tag{9}$$

where $\boldsymbol{n}$ means the vector of unit normal to the matrix/particle interface. Scalar product of vectors $\boldsymbol{c}^k, \boldsymbol{n}$ is used here.

2.3 Recovery

Recovery represents a process during which the dislocation density decreases due to annihilation of dislocation dipoles or shortening of dislocation lines. The majority of models of recovery are designed for non-reinforced materials in which the dislocations form subgrain boundaries. The models are summarized in [12]. A closed connection with recovery in superalloys can be found in the paper by Mukherji and Wahi [13] dealing with climb of dislocations on the matrix/particle interface. The climb resistance is described by a factor given by the increase of the dislocation length due to dislocation climb over the particle. The model does not involve the kinetics of climbing. During the recovery the dislocation loops move nonconservatively along the matrix/particle interface to places where the loops can shrink and disappear. This idea has been proposed first by Dlouhý et al. on the basis of experimental and theoretical works [7, 8]. In the analysis the authors use the following simplifications: i) the process of recovery is described in a global way by a characteristic time, ii) diffusional creep connected with recovery is not taken into account.

The recent models do not offer a detailed description of recovery involving the changes of the dislocation density in time at a given point of the matrix/particle interface. Such model has been developed and it is presented in this subsection.

In our model we assume that during its nonconservative motion the whole dislocation loop always lies in its slip plane. In reality it is not true. However, if we are not interested in the exact shape of the loop, but in the global motion of the loop, the assumption is plausible. Thus, the dislocation loop is determined by the section of the slip plane with the particle surface. The position and shape of the loop is determined by one coordinate ξ^k in the direction of $\boldsymbol{c}^k$.

Let us consider a point at the dislocation loop on the matrix/particle interface having the local normal $\boldsymbol{n}$. The force $\boldsymbol{q}$ acting on the interface unit area has the components

$$q_i = \sum_{j=1}^{3} \sigma_{ij} n_j \,. \tag{10}$$

Let us consider one fixed k from $\{1, \ldots, N\}$ now. In this case the index k will be omitted. If the coordinate ξ of the loop changes by $\mathrm{d}\xi$, the point at the loop moves by the distance

$$\mathrm{d}\varphi = \frac{\mathrm{d}\xi}{\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}} \tag{11}$$

along the interface. Then the work $\mathrm{d}L$ released by moving of the loop on the account of the stress is given by

$$\mathrm{d}L = \oint \sum_{i=1}^{3} q_i \beta a_i \mathrm{d}\varphi \mathrm{d}\eta = \beta \sum_{i=1}^{3} a_i \mathrm{d}\xi \oint \frac{q_i \quad \mathrm{d}\eta}{\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}} \,, \tag{12}$$

where $\oint \ldots \mathrm{d}\eta$ is calculated as the curve integral along the whole loop. The total force F acting on the dislocation loop in the direction $\boldsymbol{c}$ follows then from the equation

$$F = \frac{\mathrm{d}L}{\mathrm{d}\xi} - \gamma \frac{\mathrm{d}}{\mathrm{d}\xi} \oint \mathrm{d}\eta = \sum_{r=1}^{3} \oint \frac{\beta \boldsymbol{a} \cdot \boldsymbol{q} \quad \mathrm{d}\eta}{\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}} - \gamma \frac{\mathrm{d}}{\mathrm{d}\xi} \oint \mathrm{d}\eta \,. \tag{13}$$

The second term in (13) expresses the change of the energy due to the change of length of the loop. The nonconservative motion of the dislocation loop involves climbing processes which are connected with diffusional transport of atoms. To move the dislocation along the interface, it is necessary to deposit a layer of atoms on the interface of the thickness $\beta \boldsymbol{a} \cdot \boldsymbol{n}$ (see [14]). Jogs at dislocations serve as only sources and sinks of atoms. We assume a certain mean distance between jogs w. If the loop moves with the velocity $\dot{\xi}$, the total diffusive flux (in m^3/s) into the jog is

$$J = w \frac{\dot{\xi}}{\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}} \beta (\boldsymbol{a} \cdot \boldsymbol{n}) \,. \tag{14}$$

The diffusion is driven on the account of the force F from (13). The diffusion is a dissipative phenomenon which changes the power $F\dot{\xi}$ into the heat. The heat production R due to the diffusive fluxes j (in m/s) is given by [15]

$$R = \frac{KT}{D\Omega} \int_V j^2 dV \,, \tag{15}$$

where D is the lattice diffusion coefficient, K the Boltzmann constant, T the absolute temperature, Ω the atomic volume and V the volume in which diffusion occurs. The decisive part of the heat is produced in the vicinity of the jog. If we suppose that the diffusion occurs in the half sphere of the radius Λ in the matrix around the jog (the diffusion does not occur in the particle), the diffusive flux j in the distance λ from the jog is

$$j = \frac{J}{2\pi\lambda^2} \,. \tag{16}$$

Then the heat production in the half sphere is

$$R^{\mathrm{jog}} = \frac{KT}{D\Omega} \int_{\beta}^{\Lambda} 2\pi\lambda^2 j^2 \mathrm{d}\lambda = \frac{KTJ^2}{2\pi D\Omega} \left(\frac{1}{\beta} - \frac{1}{\Lambda} \right) \approx \frac{KTJ^2}{2\pi D\Omega\beta} \,. \tag{17}$$

From this equation it follows that for the radius $\Lambda \gg \beta$ its magnitude plays negligible role in the heat production. It can be further estimated (see [14]) that the diffusive transport of atoms in the matrix to the distance of the order of size of

the particle does not contribute to the heat production significantly. Thus the heat produced by the moving dislocation loop is given by

$$R^{\text{loop}} = \frac{1}{w} \oint R^{\text{jog}} \mathrm{d}\eta = \frac{KTw\dot{\xi}^2}{2\pi D\Omega\beta} \oint \frac{(\boldsymbol{a}\cdot\boldsymbol{n})^2 \quad \mathrm{d}\eta}{1-(\boldsymbol{c}\cdot\boldsymbol{n})^2} \,. \tag{18}$$

The rate $\dot{\xi}$ describing the motion of the loop can be expressed from the condition of energy conservation: the power produced by the force F dissipates into the heat R^{loop}, i.e.

$$F\dot{\xi} = R^{\text{loop}} \tag{19}$$

or

$$\dot{\xi} = \left(\oint \frac{\beta \boldsymbol{a}\cdot\boldsymbol{q} \quad \mathrm{d}\eta}{1-(\boldsymbol{c}\cdot\boldsymbol{n})^2} + \gamma \frac{\mathrm{d}}{\mathrm{d}\xi} \oint \mathrm{d}\eta \right) \Big/ \left(\frac{KTw}{2\pi D\Omega\beta} \oint \frac{(\boldsymbol{a}\cdot\boldsymbol{n})^2 \quad \mathrm{d}\eta}{1-(\boldsymbol{c}\cdot\boldsymbol{n})^2} \right) . \tag{20}$$

It is necessary to point out that the assumption about the loop remaining during its motion in the slip plane implies the fact that the total volume of atoms collected at the loop equals the total volume of atoms deposited at the loop. In other words, the motion of the loop does not require any extra sources or sinks of atoms. The assertion can be proved by the following reasoning, which assumes that the dislocation loop can move in two ways:

1. by the above mentioned nonconservative motion,
2. by shrinking of the loop by slip and expansion of another loop in another slip plane.

The second way represents two parallel cuts of the particle which do not require any extra source of atoms. Thus, also the first way cannot require any extra source of atoms.

In the reality, all dislocations need not form whole loops around the particle; in some cases only a dislocation segment can be in contact with the particle. Phenomenologically this can be expressed by the fact that dislocation density ρ varies along the section of the interface with the slip plane. Also in this general case it is reasonable to assume that between two slip planes the number of atoms remains constant. This has the consequence that in places with low dislocation density the dislocation must move along the interface quicker than in places of high dislocation density.

Let us introduce the number v of dislocations going through the slip plane in one second. The rate v depends on the coordinate ξ; v is constant around the particle for a given ξ. The relative displacement rate $\Delta\dot{\boldsymbol{u}}$ between the matrix and the particle due to the nonconservative motion of dislocations connected with deposition or collection of atoms on the interface is

$$\Delta\dot{u}_i(\xi) = \beta v(\xi) a_i \,. \tag{21}$$

The work of the forces on the interface per second in the area between ξ and $\xi + \mathrm{d}\xi$ is

$$\mathrm{d}P^{\mathrm{stress}} = \mathrm{d}\xi \oint \frac{\boldsymbol{q} \cdot \Delta\dot{\boldsymbol{u}} \quad \mathrm{d}\eta}{\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}}. \tag{22}$$

The decrease of energy of dislocations per second due to the change of length of dislocations is

$$\mathrm{d}P^{\mathrm{disl}} = -\gamma v \mathrm{d}\xi \frac{\mathrm{d}}{\mathrm{d}\xi} \oint \mathrm{d}\eta\,. \tag{23}$$

The expression $\frac{\mathrm{d}}{\mathrm{d}v}(\mathrm{d}P^{\mathrm{stress}} + \mathrm{d}P^{\mathrm{disl}})$ represents the driving force for the motion of dislocations between slip planes characterized by ξ and $\xi + \mathrm{d}\xi$. To evaluate the heat production, it is necessary to calculate the total flux into each jog at dislocations. It is given by (14) where $\dot{\xi}$ is replaced by $v\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}/\rho$. The heat production corresponding to one jog is then

$$R^{\mathrm{jog}} = \frac{KT\beta w}{2\pi D\Omega\rho^2}(\boldsymbol{a} \cdot \boldsymbol{n})^2 v^2\,. \tag{24}$$

The total heat production in the volume between ξ and $\xi + \mathrm{d}\xi$ is

$$\mathrm{d}R = \frac{\mathrm{d}\xi}{w} \oint R^{\mathrm{jog}} \frac{\rho \quad \mathrm{d}\eta}{\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}} = \frac{KT\beta w v^2 \mathrm{d}\xi}{2\pi D\Omega} \oint \frac{(\boldsymbol{a} \cdot \boldsymbol{n})^2 \bullet \mathrm{d}\eta}{\rho\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}}. \tag{25}$$

From the condition

$$\mathrm{d}P^{\mathrm{stress}} + \mathrm{d}P^{\mathrm{disl}} = \mathrm{d}R \tag{26}$$

v can be evaluated; it results

$$v = \frac{2\pi D\Omega}{KT\beta w}\left(\beta \oint \frac{\boldsymbol{a} \cdot \boldsymbol{q} \quad \mathrm{d}\eta}{\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}} - \gamma \frac{\mathrm{d}}{\mathrm{d}\xi} \oint \mathrm{d}\eta\right) / \oint \frac{(\boldsymbol{a} \cdot \boldsymbol{n})^2 \quad \mathrm{d}\eta}{\rho\sqrt{1 - (\boldsymbol{c} \cdot \boldsymbol{n})^2}}. \tag{27}$$

For dislocations from N slip systems, the relative displacement rate between the matrix and the particle is given (see (21)) by

$$\Delta\dot{u}_i(\xi) = \sum_{k=1}^{N} \beta v^k(\xi) a_i^k\,. \tag{28}$$

From the continuity equation it follows that the rate of a decrease of the dislocation density due to recovery is given by

$$\dot{\rho}^{k-} = \frac{\mathrm{d}v^k}{\mathrm{d}\xi}\sqrt{1 - (\boldsymbol{c}^k \cdot \boldsymbol{n})^2}\,. \tag{29}$$

3. Outline of the model

The model solves the cooperation of elasticity, time-dependent crystal plasticity and recovery of the dislocation structure on the matrix/particle interface. The matrix and the particles can have different elastic constants and different parameters of the crystal plasticity. In this paper no plasticity in the particles is assumed. Further, it is supposed that internal stresses exist in the composite.

Immediately after the application of the external load the dislocation densities on the matrix/particle interfaces are taken to be zero and the stress state is determined by elasticity as the superposition of the external stress and the internal stress. The internal stress is represented by coherency stress in case of superalloys or by thermal stress in case of metal matrix composites. The stress in the matrix determines the slip rate in the matrix (see (5)) and the rate of generation of dislocations on the matrix/particle interface (see (6)). The actual stress state and the actual dislocation densities on the interface determine the rate of recovery. Recovery leads to a decrease of the dislocation density (see (29)) and to a relative displacement between the matrix and the particle (see (28)). Thus, the rate of change of the dislocation density on the interface for the k^{th} slip system is given by

$$\dot{\rho}^k = \dot{\rho}^{k+} - \dot{\rho}^{k-}; \tag{30}$$

ρ^{k+} and ρ^{k-} are given by (9) and (29), respectively. In the steady state the terms $\dot{\rho}^{k+}$ and $\dot{\rho}^{k-}$ are compensated and the dislocation density no longer depends on time.

4. Mathematical solution

The mathematical solution of the problem required to develop an original mathematical approach and the FEM code based on small strain approximation. The mathematical treatment cannot be completely described in this paper; some formulations and results have been presented in [16], the more detailed study on the solution of this problem including existence and convergence theorems will be published in the specialized journal [17].

The general approach is based on the integral formulation of the following five types of equations.

1. Equations of principle of virtual displacement rates for materials consisting of 2 phases (jumps in geometrical configuration at matrix/particle interfaces must be allowed). These equations involve the equilibrium conditions on the surface of the unit cell and on the matrix/particle interface and the Cauchy differential equilibrium conditions.

2. Constitutive equations for stress components, making use of the serial Maxwell model with one linear elastic and one nonlinear viscous parts. The linear

elastic part is given by the Hooke law for cubic crystals with the well-known elastic constants C_{11}, C_{12} and C_{44}. Then for any $i = 1, 2, 3$

$$\dot{\sigma}_{ii} = C_{11}(\dot{e}_{ii} - \dot{\varepsilon}_{ii}) + (1 - \delta_{ij})C_{12}(\dot{e}_{jj} - \dot{\varepsilon}_{jj}) \tag{31}$$

and for any $i, j = 1, 2, 3$ such that $i \neq j$

$$\dot{\sigma}_{ij} = C_{44}(\dot{e}_{ij} - \dot{\varepsilon}_{ij}) \tag{32}$$

hold; in these relations $\underline{\dot{e}}$ is the total strain rate tensor and $\underline{\delta}$ the Kronecker symbol. It can be verified (see [18]) that in orthogonal decomposition of the total stress tensor $\underline{\sigma}$ into the volumetric and deviatoric components only the constitutive equations for deviatoric components are nonlinear.

3. Compatibility conditions for geometrical configuration on the matrix/particle interfaces expressed by (28).

4. Equations for the kinetics of the displacement between the matrix and the particle due to recovery given by (27).

5. Equations for the evolution of the dislocation density described by (30).

The derived system of integral equations is of hyperbolic type, but it can be analyzed as the system of equations of evolution using the Rothe method of discretization in time. This makes it possible to convert our problem into the searching for solutions of certain sequences of more simple time-independent systems. Such systems can be analyzed by means of the FEM; some nonstandard techniques must be applied to handle the unknown contact loads and the geometrical discontinuities on the matrix/particle interfaces. Since no appropriate FEM code suitable for our purpose has been known to the authors, the original software package CDS for PC's and workstations in C++ language has been developed.

5. Numerical example and discussion

Let us consider a simple periodic 2-D material structure consisting of square particles of size 0.45 μm separated by matrix channels of the thickness of 0.05 μm. Such dimensions are typical for superalloys. Due to symmetry of the structure the area $0 \leq x_i \leq 0.25\,\mu$m $(i = 1, 2)$ can be used as a unit cell. The structure is assumed to be independent on the x_3 coordinate.

The structure is loaded by external tensile stress in x_2 direction. Moreover the initial volumeric strain of magnitude -10^{-3} is present in the particle. This strain introduces the same internal stress into the composite as that caused by misfit -10^{-3} and zero density of misfit dislocations at the interface.

The elastic constants in both materials (see (31) and (32)) are used for the simplicity the same: $C_{11} = 18 \times 10^{10}$ Pa, $C_{12} = 12 \times 10^{10}$ Pa, $C_{44} = 10 \times 10^{10}$ Pa.

For the slip in the matrix channels (see (6)) the parameters $A = 5 \times 10^{-11}\,\mathrm{Pa/s}$, $n = 1$ and $\tau^k_{\mathrm{Orowan}} = 1.5 \times 10^8\,\mathrm{Pa}$ $(k = 1, 2)$ are used. Two slip systems are assumed characterized by unit vectors $\boldsymbol{a}^1 = \boldsymbol{c}^2 = (-1/\sqrt{2}, 1/\sqrt{2}, 0)$ and $\boldsymbol{a}^2 = \boldsymbol{c}^1 = (1/\sqrt{2}, 1/\sqrt{2}, 0)$. The magnitude of the Burgers vector is $\beta = 2.5 \times 10^{-10}\,\mathrm{m}$. The typical value of the diffusion factor in the expression for recovery (see (27)) $d = 2\pi D\Omega/(KTw\beta)$ is set to $2.4 \times 10^{-7}\,\mathrm{m^3 s^{-1} J^{-1}}$. The value of the factor corresponds to the coefficient of autodiffusion in the matrix at the temperature 850 °C and $w = 30\beta$. The choice of γ in (27) is not substantial in our cases.

For an arbitrary time all strains, stresses, dislocation densities, and displacement rates related to the initial geometric configuration can be expressed as functions of coordinates x_1 and x_2 (except displacement rates in x_3 direction that are linear functions of x_3).

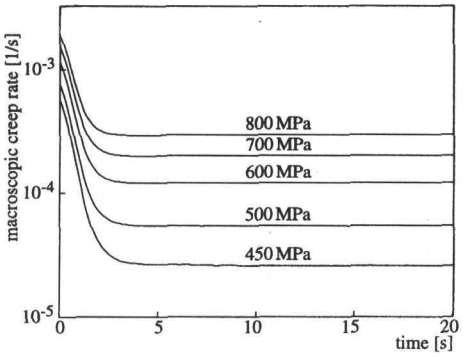

Fig. 1. Creep rate for different applied stresses.

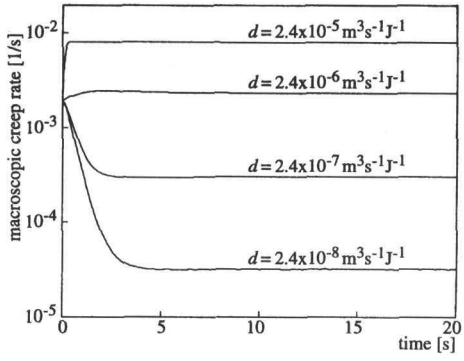

Fig. 2. Creep rate for different diffusion factors d.

Fig. 1 demonstrates the time evolution of the creep rate for different applied stresses from the interval $\langle 450, 800\rangle$ MPa. In Fig. 2 the creep rates were calculated for different diffusion factors $d \in \langle 2.4 \times 10^{-8}, 2.4 \times 10^{-5}\rangle\,\mathrm{m^3 s^{-1} J^{-1}}$ and the applied stress 800 MPa. From the figure it can be seen that for the diffusion factor $d \leq 2.4 \times \times 10^{-6}\,\mathrm{m^3 s^{-1} J^{-1}}$ the steady state creep rate is nearly proportional to the diffusion factor; the diffusion is the controlling mechanism of creep. However, the diffusion is connected with recovery and, thus, creep under these conditions can be called the recovery controlled creep.

In the work by Svoboda and Lukáš [14] a simple model of the recovery controlled creep has been developed. The model assumes that the stress states within the whole particle and within the matrix channels of both types (normal and parallel to the applied stress) are homogeneous. For the steady state this assumption is confirmed by the present paper.

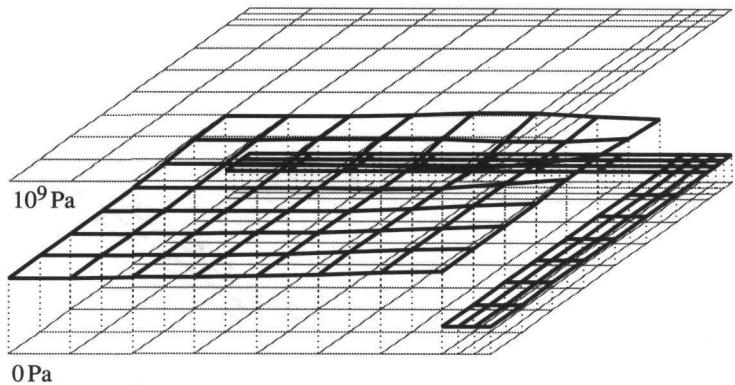

Fig. 3. Resolved shear stress $\tau^1 = \tau^2$.

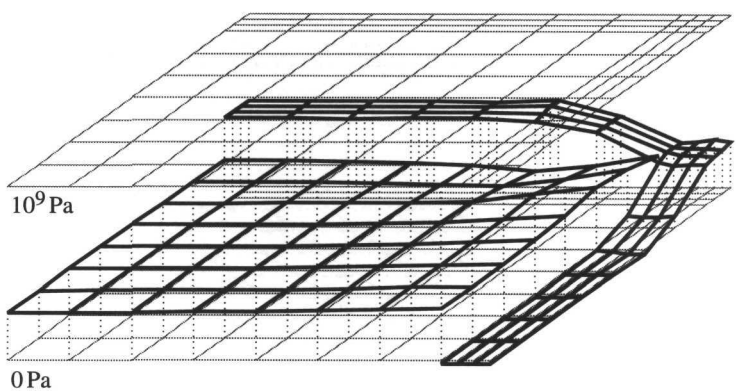

Fig. 4. Hydrostatic stress $\sigma_H = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33})$.

In Fig. 3 the distribution of the resolved shear stress $\tau^1 = \tau^2$ (see (1) in the steady state creep) is plotted for the particle and the channels. The results are for the applied stress 800 MPa and $d = 2.4 \times 10^{-7}\,\mathrm{m^3 s^{-1} J^{-1}}$. The distribution of the hydrostatic stress is shown in Fig. 4. Analogously the distribution of other components can be plotted. It can be concluded that the stresses in the mentioned areas can really be treated as homogeneous and the assumption on stresses done in [14] is plausible.

The displacement rates in the x_1 and x_2 directions in the steady state creep are shown in Fig. 5 and 6. Two facts follow from these figures:

- The rate of plastic strain due to slip is homogeneous in the matrix.

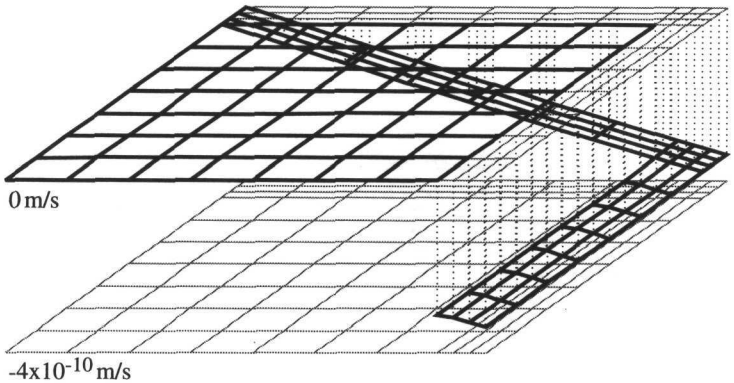

Fig. 5. Displacement rate, x_1-direction.

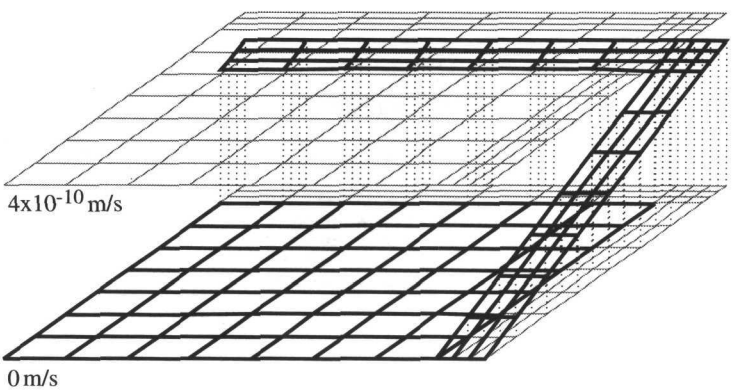

Fig. 6. Displacement rate, x_2-direction.

- Jumps in the displacement rates at the matrix/particle interface can be seen. These jumps are due to recovery. During the motion of dislocations along the matrix/particle interface the atoms at the interface parallel to the applied stress are collected, transported by diffusion and deposited at the interface normal to the applied stress. The motion of the dislocations also causes the sliding along the interface.

The kinetics of recovery in the model [14] was derived under the assumption that the dislocation densities at the interfaces normal or parallel to the applied stress are homogeneous.

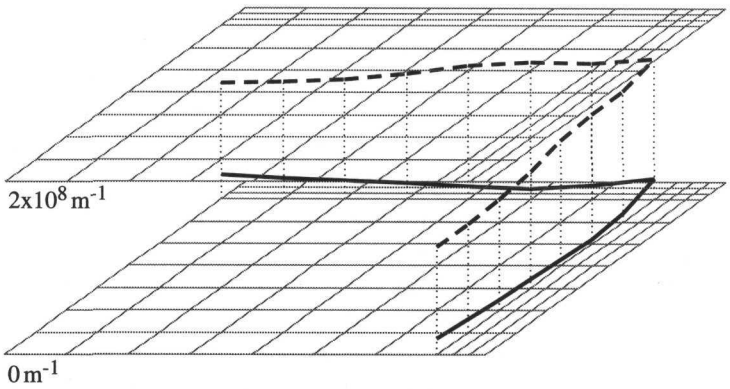

Fig. 7. Dislocation density ρ^1 (full line), density of dislocations generated by slip (dashed line).

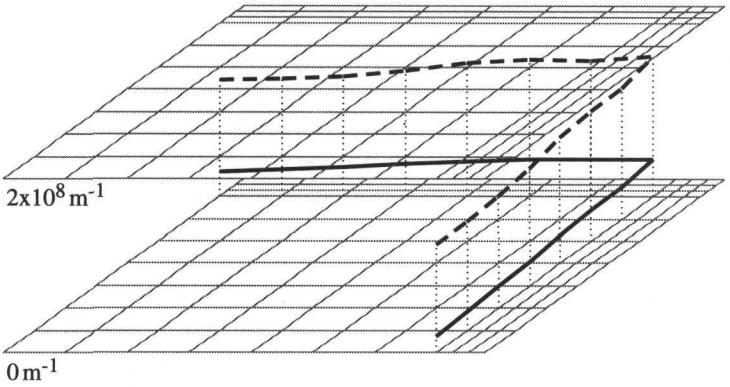

Fig. 8. Dislocation density ρ^2 (full line), density of dislocations generated by slip (dashed line).

Figs. 7 and 8 offer the full description of the dislocation densities at the interface. Due to the symmetry, the dislocation density of one of the slip system is symmetric along both axes x_1 and x_2 with the dislocation density of the other slip system. The dashed lines in these figures correspond to the densities of dislocations generated by slip in the matrix channels during 80 s after the loading. The inhomogeneities in the dislocation densities are not negligible. In comparison with the simple model [14] assuming constant dislocation densities on particular interfaces, the present model gives the rate of recovery slightly lower. However, the difference

seems to be unimportant, as the exact values of the diffusion coefficient D and of the mean jog distance w are not available.

The results of recent FEM modelling [5, 6] and the present FEM modelling differ substantially in the stress distribution and in the field of displacement rates. The results of recent FEM models assuming the viscoplastic flow of the matrix show the development of pressure gradients in the whole matrix and the shearing of the matrix along the matrix/particle interfaces. On the other hand, our results show practically constant pressure (see Fig. 4) in particular matrix channels (with a "jump" near the particle corner) and the homogeneous plastic strain rate in the matrix (see Fig. 5 and 6). The incompatibility between the plastic strain rate in the matrix and zero strain rate in the particle is compensated by collection and deposition of atoms at the matrix/particle interfaces and by sliding along the matrix/particle interfaces which are the direct consequences of the recovery.

6. Conclusions

The model of creep in composites taking into account the crystallographic slip in the matrix and dynamic recovery is presented. The paper is based on the following items:

1. The matrix of the composite deforms by time dependent crystal plasticity. The equations for the rate of deposition of the dislocations from individual slip systems at each point of the matrix/particle interface have been derived.

2. The quantitative description of recovery of dislocations deposited on the matrix/particle interface due to nonconservative motion of dislocations along the interface has been developed. The driving force of recovery is a function of the local stresses on the interface and of the particle geometry. The recovery is controlled by lattice diffusion dissipating the work of the driving force.

3. The mathematical approach solving the problem of the elasticity and the time-dependent crystal plasticity and recovery has been developed. The mathematical approach is based on integral formulation of the problem which is suitable for the solution by FEM.

4. As the commercial FEM packages are not designed to solve such problems, an original FEM code has been developed in the framework of our research activities.

5. The FEM code is applied to the modelling of creep in superalloys. The results are significantly different from the results of recent FEM modelling.

Acknowledgement

This paper is based on the research in the frame of COST-512 action supported by the Czech Ministry of Education (project OC-COST 512-10). The authors thank Prof. P. Lukáš (IPM, CZ) and Prof. G. Eggeler (IEM, DE) for reading the manuscript and for critical comments.

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Received: 23.9.1997

Appendix

Connection between slip in the matrix and generation of dislocations on the matrix/particle interfaces

For a fixed k^{th} slip system ($k = 1, \ldots, N$) let us consider the vectors $\boldsymbol{a}^k$ and $\boldsymbol{c}^k$ and the corresponding tensor $\underline{b}^k$ from (8). Then the tensor of plastic deformation $\underline{\varepsilon}^k$ has the components (for $i, j \in \{1, 2, 3\}$)

$$\varepsilon_{ij}^k = \bar{\varepsilon} b_{ij}^k \,. \tag{A1}$$

The slip deformation $\bar{\varepsilon}$ is due to discrete slips by Burgers vector β in the slip planes of the distance p where

$$p = \frac{\beta}{\bar{\varepsilon}} \,. \tag{A2}$$

Since $\boldsymbol{n}$ is the unit vector normal to the interface where the dislocations remain deposited, the distance s between dislocations is given by

$$s = \frac{p}{\sqrt{1 - (\boldsymbol{c}^k \cdot \boldsymbol{n})^2}} \,. \tag{A3}$$

The dislocation density ρ^k on the interface is then

$$\rho^k = \frac{1}{s} = \frac{\bar{\varepsilon}}{\beta} \sqrt{1 - (\boldsymbol{c}^k \cdot \boldsymbol{n})^2} \,. \tag{A4}$$

Differentiating (A4) in time and putting this result together with (6) and (A1) gives (9).