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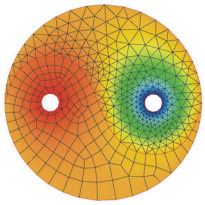

APPLICATION OF COMBINED DISCRETE/FINITE ELEMENT MULTISCALE METHOD FOR MODELLING OF Mg REDISTRIBUTION DURING HOT ROLLING OF ALLUMINIUM

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Abstract

Numerical modelling of the stock surface layer formation has been carried out to support simulations of the reheating and breakdown rolling of the Al-Mg-Mn aluminium alloy AA3104 using a two-high laboratory mill. The results of the experimental programme have demonstrated that the structure, morphology and the filiform corrosion susceptibility of the subsurface layer appears to be strongly dependent on both the depth of the Mg enrichment formed during reheating and redistribution of this near-surface metallic element during hot rolling. The numerical problem became effectively a matter of discrete rather then continuum numerical analysis. The applied combined finite-discrete element method merges finite element tools and techniques with discrete element-based transient dynamics, contact detection and contact interaction solutions. Linking of the modelling scales is based on transferring of the corresponding boundary conditions from the macro model to the representative cell, considered as the meso- level model. This meso- model consists of a large number of deformable bodies that interact with each other. Each individual discrete element is of a general shape and size, and can be discretised into finite elements to analyse deformability and diffusion. The transfer processes in the thin surface layer are described by the system of diffusion and the motion equations for particles integrated in time. The numerical analysis indicated that, under the rolling conditions, the redistribution of Mg content can arise mainly due to one or a few of the following reasons, namely: by removal of some of the thin oxide layer by abrasion and adhesion to the work roll surface; by intermixing of the small oxides (Mg) into the subsurface layer of a few microns depth; and by diffusion. Further analysis should be carried out to validate the modelling approach and to establish the predominant mechanisms of the surface layer formation and influence of the key hot rolling parameters.

Key words: alluminium hot rolling, multiscale numerical analysis, combined finite-discrete element method, oxides, surface quality, deformation

1. INTRODUCTION

The mechanisms and processes involved in the formation of the thin (a few microns) subsurface layers in hot rolled aluminium flat products are of considerable interest to the aluminium industry. The effect of these remarkably fine subsurface layers on product quality, and in particular, on resistance of the surface to subsequent filiform corrosion has been observed a few years ago [6] and further understanding of the role of these layers has been developed recently [1, 9]. It is believed that the tribological conditions at the roll/stock interface during processing, such as state of lubrication, position of the neutral point, roughness of the rolls and the roll speed, are primarily responsible. However, there has not been a systematic investigation of the influence of rolling conditions on the formation of the subsurface layers and the present paper presents the potential of the modelling approach based on application of the

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latest modelling technology including combined discrete/finite multiscale method developed to support the experimental programme.

2. MORPHOLOGY OF THE SURFACE LAYER

A surface layer of hot rolled Al-Mg alloys consists of about 10-160 nm thick layer of continuous metal oxides followed by a subsurface layer of 1.5 – 8 μm thick (figure 1) [2]. The subsurface layer consisted mainly of small grained metal with grain boundaries pinned by 2.5 to 50 nm crystalline and amorphous oxides. The oxide type depended on the process stage, with MgO, γ-Al_2O_3 , $MgAl_2$ and amorphous Al_2O_3 observed at the start of the process, while only MgO found at the end stage. This is associated with the decrease in processing temperature. Grain growth in the subsurface layer was retarded by Zener pinning by small oxide particles. For aluminium AA3XXX alloys, the most significant microstructural feature influencing filiform corrosion susceptibility appeared to be redistribution of intermetallic particles in the significantly deformed subsurface layer, which results in finer intermetallic particles in this region compared to the initial material [9].

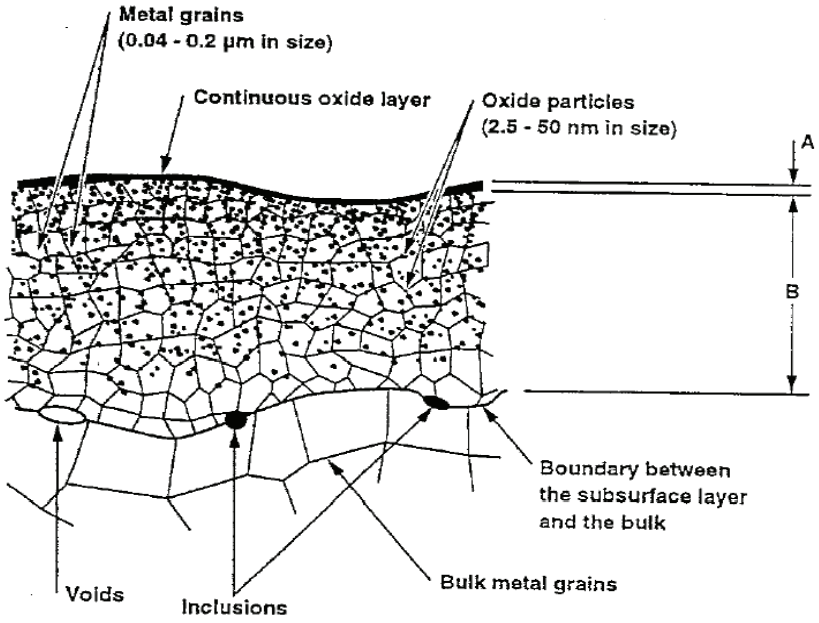

Fig. 1. Schematic representation of the surface layer containing microcrystalline oxides mixed with small grained metal and covered with a continuous layer of surface oxide [2].

3. BASIC ASSUMPTIONS OF THE NUMERICAL APPROACH

One of the assumptions of the modelling approach is that both the frictional force and wear at the surface layer result from the interaction between significantly harder asperities of the roll and softer material of the stock during rolling passes. The condition that is applied in hot rolling of aluminium alloys. In this case the energy produced by sliding is dissipated mainly by plastic deformation of the surface layer, by shearing and failure taking place near the stock surface. Following the above representation initially developed for characterisation of metallic sliding friction mechanics by Kopalinsky and Oxley [4], the following assumptions has been made for this combined numerical approach. It is combined discrete element (DE) and traditional finite element (FE) method together. The FE analysis is used for macro-scale simulation while the DE method is applied to simulate meso-scale phenomena taking place in the surface layer of a few micron thickness. In such way, the meso- model is reduced to a representative cell at the stock-roll interface. Load histories for the cell are taken from the macro-model. The design of the representative cell is based on the inputs from the experimental studies [3]. The cell is composed of a central part that is the mesoscopic cell containing morphological features of the interface such as roll asperities, failed scale fragments, debris, voids, etc.; and a surrounding part called the transition zone. The transition zone allows a homogeneous stress, strain and temperature fields to be obtained around the representative cell in order to compare them with the real values in the experimental testing.

4. COMBINED METHOD, REPRESENTATIVE CELL AND TRANSITION ZONE

The numerical method applied in this work is a combined method. It combines two different scales of modelling, such as macro- and meso-, and also, it combines finite element analysis of a continuum with a discrete element dynamic method applied for the simulation of meso-scale particulate phenomena. The approach uses both the discrete element method at meso-scale to reach the necessary precision, and the finite element method at macro-scale to save the computational resources. Although particle models for studying micromechanics of materials should wait until

computer power becomes sufficient, this work is an example of experimentation with the methodology. The model is developed in 2-D to keep the computational resources reasonably small. Figure 2 illustrates the macro- model setup including 3 consecutive rolling passes assuming plane strain conditions. The model enables calculation of the distributions of velocities, strains, strain rates, stresses and temperature around the representative deformation zone near the surface of the rolled material, in such way allowing the load histories to be taken for the representative cell. The mechanical and thermal properties of the material were assumed to be similar to those used in rolling models. The representative cell together with the transition zone is illustrated schematically in figure 3. The meso- model consists of a large number of bodies that interact with each other. Each individual discrete element is of a general shape and size. The discrete elements can be introduced into the model as a set of rigid bodies. They can also be deformable and are discretised into finite elements to analyse deformability and diffusion [7].

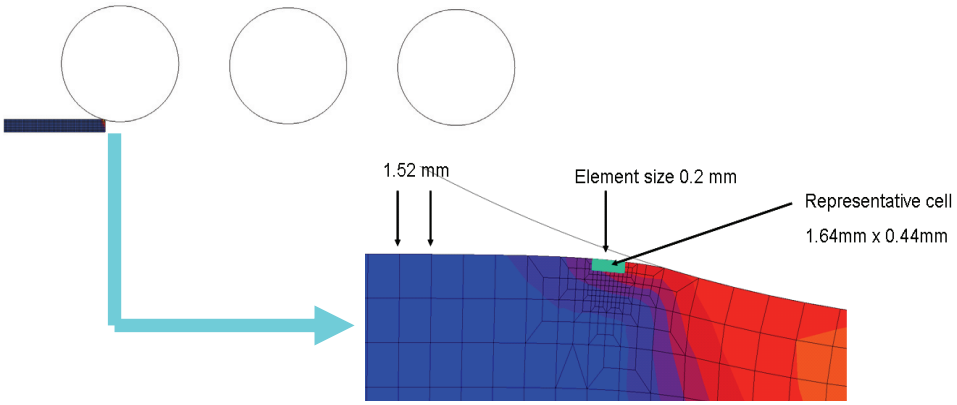

Fig. 2. Schematic representation of the macro- model setup.

The basic assumption of the discrete analysis is that a solid material can be represented as collection of particles/blocks interacting among themselves in the normal and tangential directions. The motion of each element is governed by Newton's law as:

$$m_i \ddot{u}_i = F_i + F_i^{damp}, \qquad I_i \dot{\omega} = T_i + T_i^{damp} \quad (1)$$

where u is the element centroid displacement in a fixed coordinate frame; ω is the angular velocity; m is the element mass; I is the moment of inertia. Vectors F and T correspondingly are the resultant of all forces and moments applied to the i-th element due to external load, contact interactions with neighbouring blocks and other obstacles.

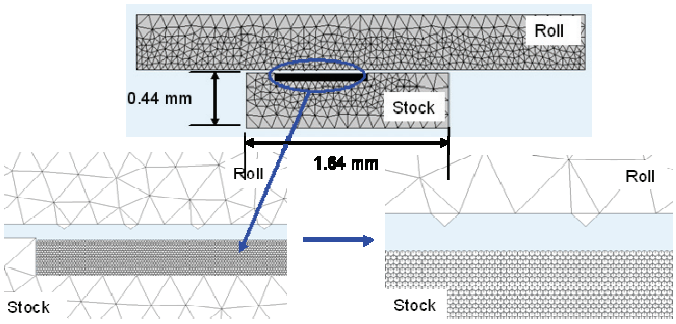

Fig. 3. Schematic representation of the meso- model setup.

The contact forces between two blocks are decomposed into normal and tangential components and obtained using a constitutive model formulated for the contact. A quasi-static state of equilibrium of the assembly of blocks is achieved by application of non-viscous type damping necessary for kinetic energy dissipation:

$$F_i^{damp} = -\alpha^t \|F_i\| \frac{\dot{u}_i}{\|\dot{u}_i\|}, \quad T_i^{damp} = -\alpha^r \|T_i\| \frac{\omega_i}{\|\omega_i\|} \quad (2)$$

where α^t and α^r are damping constants for translational and rotational motion respectively. Initial bonding for the neighbouring particles can also be assumed.

The main assumption of the finite element method is that continuum domain is discretised with finite elements. Combining discrete and finite element methods involves treatment of contacts between discrete particles/blocks and finite element edges. Similarly to the case of contact between two spheres, the contact force between the sphere and external edge of a finite element is decomposed into normal and tangential components and generally can include cohesion, friction, damping, heat generation and exchange [8]. To obtain continuity in transferring mechanical and physical variables between discrete and finite element zones, a transition zone can also be introduced between those domains. The idea of the transition zone is that the domain is discretised and governed by both discrete and finite element methods [10]. In this zone, the thickness of which can be adjusted to obtain the necessary level of smoothness, the loca-

tion of the discrete elements is constrained by the location of the relative finite element nodes. It allows the continuity of the displacements, strains and stresses in the domain. The algorithm for the transient dynamic problem involving both discrete and finite elements includes cyclic consecutive computation of the nodal velocities, the nodal displacements, the nodal pressures, updating the nodal coordinates, checking the frictional contact forces and updating the residual force vector. It is realised using both MSC Marc and ELFEN commercial software. The critical time step for the entire calculation is taken assuming the critical time step for the discrete analysis, which is much smaller than the one for the finite element analysis.

Assuming a constant temperature T, the transfer processes within the thin subsurface layer can be described by the system of diffusion and the motion equations (1), (2) and (3) for particles integrated in time using a central difference scheme:

$$\frac{\partial}{\partial x}\left(D(T)\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D(T)\frac{\partial C}{\partial y}\right)=\frac{dC}{dt}$$
$$C=C(x,y,t);\quad 0\le x\le L_x;\quad 0\le y\le L_y;\quad t>0. \tag{3}$$

where $D(T)$ is the diffusion coefficient; C is the concentration and t is the time. In such a case, the amount of substance transferring across the area, and governed by the system of equations (2) and (3), is expected to be significantly different from what it should be assuming that only diffusion process responsible for the transfer depending on the extent of mechanical mixing in the area.

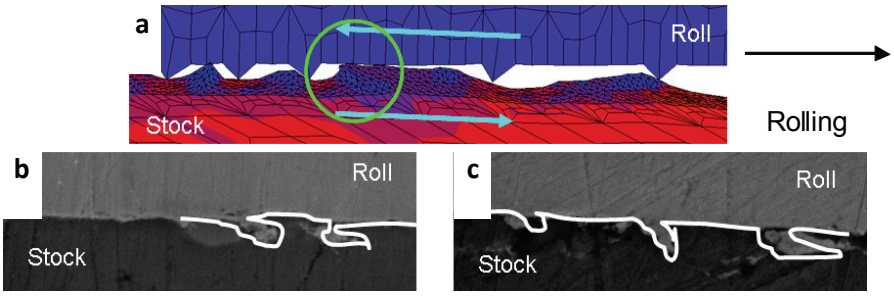

Fig. 4. *Profile of the stock surface layer during hot rolling of aluminium formed due to relative slip at the roll/stock interface. Prediction (a) and SEM images (b, c).*

5. SIMULATION OF THE PHENOMENA RESPONSIBLE FOR FORMATION OF THE STOCK SURFACE LAYER

Adoption of the mechanical model of metallic sliding friction allowed for numerical representation of a wide range of the phenomena responsible for formation of the stock surface layer during hot rolling of aluminium arising from slip at the roll/stock interface and the action of roll surface imperfections on the stock surface. It has been shown earlier that it is possible to investigate the influence of a range of the technological parameters, such as rolling direction, aspect ratio, roll roughness and rolling speed on mechanical churning in the area using multi-scale continuum finite-element model [5]. Figure 4 illustrates the effect of the forward and backward slip on formation of the "churned" profile of the stock surface. The arrows (figure 4 a) indicate the relative slip between the "hard" roll and the "soft" stock surface near the exit from the roll gap. The highlighted lines (figure 4 b and c) exhibit the observed profile of the workpiece surface, which is similar to the predicted one. It has been shown that the churning depends on the yield stress in the area. The lower the assumed yield stress of the surface layer, the less is the tendency for churning. It has to be noted that the mechanical properties of this very thin surface layer of the aluminium alloy can be significantly different from the material bulk properties and this effect is the subject to further research. In addition to this, application of the developed combined discrete/finite element model allows for prediction of the mechanical mixing in the thin subsurface layer on a meso-scale level due to the specific tribological conditions in the roll gap (figure 5). The predicted displacements both in vertical (Y) and horizontal (X) directions allow for the assumption that the particles can be displaced at least on the distance comparable with the size of the roll asperities and intermixed in the layer. As can be seen in figure 6, the numerical approach allows diffusion between the discrete element blocks that are discretised into finite elements in this case, to be taken into consideration. The concentrations of 13-14 particles chosen randomly at the same depth within the surface layer are plotted versus corresponding depths for the different time during the rolling pass. Figure 6 illustrates a typical trend in the Mg redistributions predicted in the surface layer of the aluminium stock. The progressive increase of the scatter illustrates the role of the mechanical mixing in the combined mass transfer. The effect of the mixing becomes more pro-

nounced towards the end of the rolling pass that finds its reflection in the concentration profiles. Further work is needed to validate the model predictions with the measured Mg distributions during different stages of the rolling process.

thin stock surface layer during hot rolling of aluminium alloys gives the possibility for linking technological parameters, with the fine mechanisms taking place within the surface layer at the meso level, such as diffusion, churning, and mechanical mixing cou-

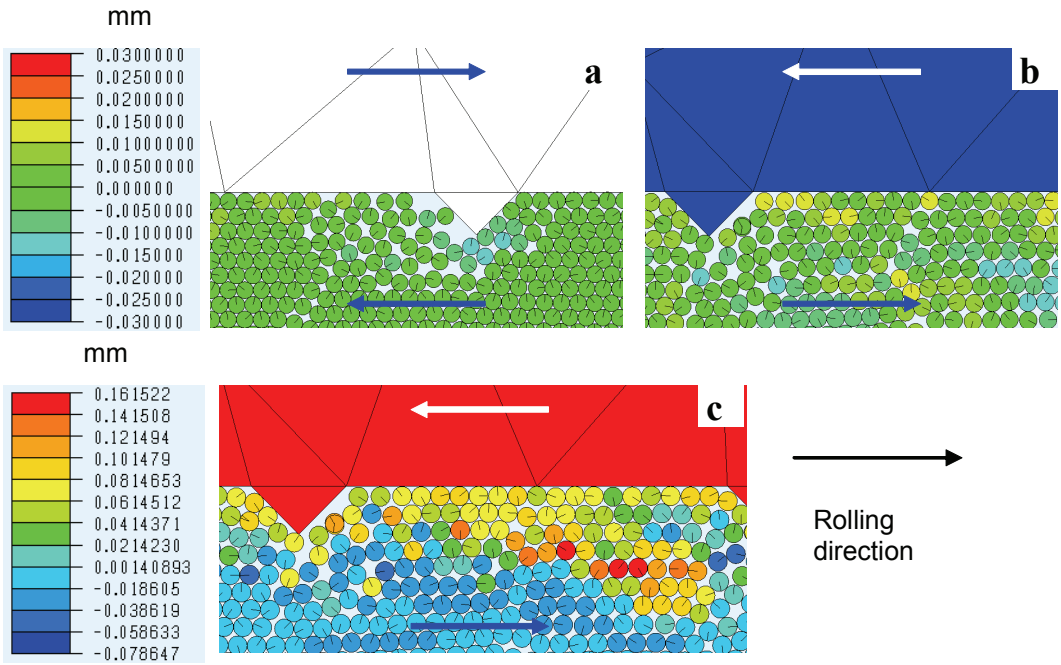

Fig. 5. Displacement of the discrete element particles/blocks in Y (a, b) and in X (c) direction predicted in the subsurface layer during hot rolling of aluminium.

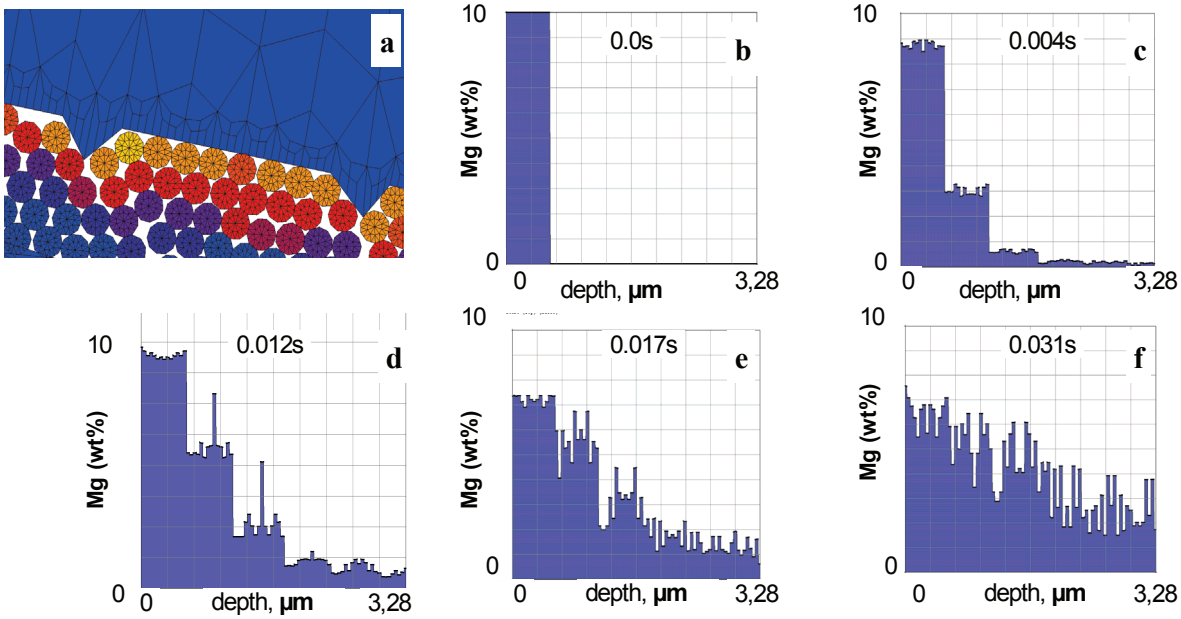

Fig. 6. Displacement of the discrete element blocks (a) and Mg redistribution in the surface layer illustrated as Mg content plotted versus depth for the different time moments (b-f) predicted during hot rolling of aluminium.

6. FINAL REMARKS

The presented numerical method for analysis of physical phenomena responsible for formation of the

pled with the heat transfer. It has been shown already that these mechanisms have significant impact on structure, thickness of the subsurface layers and the subsequent effect on filiform corrosion and they arise from slip at the roll/stock interface and the

action of roll surface imperfections on the stock surface. The developed numerical approach allows for a systematic investigation of these relations that would lead to a new level of the material understanding and design.

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ZASTOSOWANIE WIELOSKALOWEGO MODELU ŁĄCZĄCEGO METODY DYSKRETNE I ELEMENTÓW SKOŃCZONYCH DO MODELOWANIA REDYSTRYBUCJI MG PODCZAS WALCOWANIA NA GORĄCO ALUMINIUM

Streszczenie

Opracowany został numeryczny model tworzenia się warstwy powierzchniowej w celu symulacji nagrzewania i wstępnego walcowania na gorąco w walcarce laboratoryjnej duo stopu Al-Mg-Mn (AA3104). Wyniki badań doświadczalnych wykazały, że struktura, morfologia oraz podatność warstwy przypowierzchniowej na nitkowatą korozję zależą mocno od głębokości warstwy bogatej w Mg i od redystrybucji tego metalicznego pierwiastka podczas walcowania na gorąco. Modelowanie tego zjawiska jest zadaniem raczej dla analizy dyskretnej niż dla numerycznego rozwiązania kontynualnego. Zastosowane w pracy podejście łączy narzędzia i techniki metody elementów skończonych z metodą dyskretną opisującą dynamikę stanów przejściowych, detekcję styku i interakcje w obszarze styku. Połączenie różnych skal w modelu opiera się na przekazywaniu odpowiednich warunków brzegowych z modelu makro do reprezentatywnych komórek, traktowanych jako model skali mezo. Ten model mezo składa się z dużej liczby odkształcalnych ciał, które wzajemnie oddziaływają na siebie. Każdy pojedynczy dyskretny element ma ogólny kształt oraz wymiar, i może być dyskretyzowany elementami skończonymi dla przeprowadzenia analizy odkształcenia i dyfuzji. Procesy transportu w cienkiej warstwie przypowierzchniowej są opisane przez układ równań dyfuzji i ruchu cząstek, które są całkowane po czasie. Numeryczna analiza wykazała że, dla pewnych warunków walcowania, wzrost zawartości Mg w wyniku redystrybucji może być wynikiem tylko jednej lub kilku następujących przyczyn: usunięcie cienkiej warstwy tlenków przez ścieranie lub adhezję do powierzchni walców; przez wymieszanie małych tlenków (Mg) w warstwie pod powierzchniowej o grubości kilku mikronów; i przez dyfuzję. Dalsza analiza powinna zostać przeprowadzona dla weryfikacji przedstawionego modelu i dla ustalenia dominujących mechanizmów tworzenia się warstwy powierzchniowej oraz wpływu podstawowych parametrów procesu walcowania na tą warstwę.

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