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High performance computing of coating–substrate systems

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Abstract

The influence of external loads on the stability of coating–substrate systems can be analysed by the finite element method. A new FEM-code, suitable for parallel computer systems with an arbitrary number of processors, has been developed and tested on different coating–substrate systems. The three-dimensional FEM discretisation of the coated tool reaches more than 800 000 elements with approximately 2 500 000 unknowns. This way, deformations and stresses caused by external loads can be computed on a microscopic scale with sufficient accuracy and detail resolution. The presented method can contribute to a better understanding of the coated tool's behaviour under specific load situations, to the development of newly designed layer systems and to the judgement about the suitability of certain layer systems and tool geometries for specific industrial applications. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Theoretical methods; Cutting inserts; Coating–substrate systems; Finite element simulation

1. Introduction

Coated tools have a higher edge life compared to uncoated ones [1], can produce a higher surface quality of the new detail [2] and are well suited for high-speed, dry and micro machining. So coating technology gained a growing importance for industrial applications. Nowadays more than three-quarters of all tools are coated with several materials and coating systems.

Recently, manufacturers of coated tools have had a lot of experience and knowledge about coating technology and well-suited material combinations for selected industrial applications available, but do not integrate numerical methods for investigating the mechanical properties of coating systems [3]. Coating optimisation is still mostly achieved by means of 'more or less inspired' trial and error approaches [4], and the development of new coating systems, especially for new advanced machining technologies, requires a series of expensive experiments [5], in which the suitability of the coated tool for the technological process, its resistance against mechanical and thermal loads and the adhesion between the different materials must be investigated, since the adhesion of substrate and coating(s) has special importance for the further optimisation of coating technology [6].

To achieve further progress in the development of new coating systems, it is desirable to combine this experimental dominated developing process with

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numerical simulations, investigating the influence of external loads on the stability of the coatings, what mainly depends on the tool's deformation state, on the resulting stress distribution inside the tool and on the adhesion–stress ratio in a surrounding of the material boundaries. These quantities are computable by three-dimensional finite element simulations.

With the presented method, deformations, strains and stresses caused in coated tools under real-use conditions will be computed with a microscopic resolution. Stresses inside and between the coating layers become available this way. The knowledge about the stress distribution inside the coated tool, combined with information about the adhesive strength between the coating layers and the tool's material, from which critical stress values can be derived, allows predictions about the robustness of the whole coating system. Thus, this approach can support developing engineers in the design of new coating–substrate systems for advanced industrial applications, like high-speed, dry or micro machining, and in the suitability judgement of just established coating–substrate systems for special use cases.

To match the high computational expense and the large storage requirements of those computations, a parallel operating FEM software and multi-processor hardware are used, since on parallel computers the runtime may be considerably reduced and the available storage is substantially enlarged.

2. FEM modelling

For many years numerical methods like FEM are widely used for stress analysis [7,8]. Coating–substrate systems (CSS) are stressed by (in general dynamic) forces and thermal loads and are influenced by other features like residual stresses or cracks, what shall be neglected within this study. Moreover, to bound the computational effort, only static forces are considered and thermal expansion and temperature-induced stresses will not be included in the presented state of the model. For the sake of a precise reflection of realistic problems in the simulations, a three-dimensional model should be used.

The process forces acting on the coated tool's surface and the clamping principle are included in the simulational model as boundary conditions for the mechanical field problem.

Material parameters, like Poisson's ratio ν and Young's modulus E, which directly influence the deformation u and the stresses σ, depend on the material's temperature T. Precise coherencies $T \to \nu\ (T)$ and $T \to E(T)$ are rarely known, in particular for hard coating materials, but even approximations based on experimentally determined single pairs of values could improve the model's accuracy. Allowing the material parameters of the mechanical field problem to be temperature-dependent, the simulations can be carried out closer to the real use case, since in most machining processes the tool's temperature differs significantly from room temperature. For example, the warm up of the cutting edge during the machining process generates approximately 1000°C in high-speed chipping. Since the tool's deformation is typically very small, any temperature changes caused by deformation-induced dissipation can be neglected and the thermo-mechanical field problem is de-coupled. After a three-dimensional temperature distribution $T(x)$ was computed from boundary values prescribed on parts of the tool's surface, $T(x)$ can be fixed and used like a parameter in the mechanical field problem to include the material parameter's temperature dependency. The required boundary data for the mechanical and for the thermal field problem can be gained from measurements under realistic technological conditions or from theoretical considerations.

Both the thermal and the mechanical field problem must be formulated and solved in a macroscopic scale, since the external loads act on macroscopic parts of the tool's surface and the resulting temperature distributions and deformations are dependent on the whole tool's geometry. Thus, the problem scale is measured in millimetres. However, the applied coating layers have a typical thickness of at most a few micrometres down to some 100 nm and are, like the tool's substrate, characterised by specific material parameters. These parameters vary within a microscopic sub-region of the tool. Whenever these parameters are temperature-dependent, the temperature distribution must be computed with a correspondingly high spatial resolution, and the stress distribution is sought with at least the same spatial resolution to allow its evaluation in the direct surrounding of the material boundary layers. Thus, the result scale is measured in micrometers. Therefore, both the whole macroscopic tool (mm scale) and the microscopic coating layers (μm scale), must be reflected by the same geometrical model and the FE cells of the computational grid must be μm- or nm-sized, at least in a surrounding of the coating layers. Since the equally spaced high resolution meshing of a tool of volume 10 mm^3 would require 10^{10} FE cells of size 1 μm^3 and would produce a FEM equation system with $\approx 3 \times 10^{10}$ unknowns (more than 250 GB just only for the solution vector!), such uniform high-resolution meshes are not only not required but would also blast available computer resources even on the most powerful hardware installations available on earth. For this reason highly graded FE meshes must be used, with μm-sized FE cells near the coatings and mm-sized cells away from it. For the sake of an acceptable condition number of the FE matrices, the changes in the size of the FE cells must be smooth and degenerating FE cells with interior angles tending to zero should be avoided.

For the sake of shortness and simplicity, thermal influences shall not be discussed in more detail in this paper. Hence, throughout the rest of this paper a static mechanical field problem will be analysed. The presented results are related to constant room temperature.

3. Parallel FEM simulation

The reachable accuracy of FEM simulations on standard hardware is basically limited by the available storage and the acceptable computing time. Even when adapting the mesh density to the accuracy requirements in an optimal manner, the dimension of the FE equation systems for three-dimensional coating–substrate simulations will reach some 100 000s or millions and the computational effort and the storage requirements are extremely large, pushing the limits of standard hardware, even when advanced storage technologies and efficient solvers for the FE matrices are used. For this reason, multi-processor hardware and parallel working software was used for the computations, since the usage of a distributed memory computer with N processors reduces the computing time to less more than the Nth part and increases the available storage to almost N times.

In the last number of years, a variety of highly specialised parallel hardware has been developed by vendors like Cray, Fujitsu/SNI, Convex and others but was mostly used at universities or governmental institutes and in but a few large enterprises only, since this kind of computer is very expensive, mostly requiring special qualified stuff and usually not well suited for standard computer applications. Aside from this expensive hardware, the concept of networked PC-clusters with the operating system LINUX is worth the money alternative. Simultaneous with the parallel task, each integrated hardware component can be used for standard applications, too, giving the owner a greater flexibility.

A mechanism for data exchange and communication is needed when more than one processor of a distributed memory machine work together on the solution of a problem. That requires a physically existing network (fast Ethernet with transfer rates of 100 Mb/s) as well as additional software components for accessing this network (MPI, **M**essage **P**assing **I**nterface [9]).

For parallel FEM applications, the dominating programming model is **D**omain **D**ecomposition (DD) [10]. For N processors, the simulational domain Ω (the tool's geometrical model) is divided into N non-overlapping subdomains Ω_i with boundaries $\partial\Omega_i$, and each processor does all the computational work related to 'its' subdomain (Fig. 1). All steps and data of the algorithm, from mesh generation, FEM assembly and solver up to the preparation of graphical post-processing may be performed and stored locally by processor P_i, with some local communication for data exchange over the coupling boundaries $\partial\Omega_i \cap \partial\Omega_j$ and some global communication for control purpose and I/O. The efficiency of the whole parallel algorithm is highly influenced by the quality of the DD: For a good load balancing, each Ω_i should contain nearly the same number of grid nodes, and the smaller the set $\cup(\partial\Omega_i \cap \partial\Omega_j)_{i \neq j}$, the smaller is the expense for the necessary data exchange. The most time and memory consuming part of the simulational program is the solver for the linear equation systems, even when sparse matrix techniques and fast solvers are used. Iterative methods should be preferred, because direct solvers show a bad error propagation and, due to the unavoidable fill-in, require too much storage when applied to large equation systems. Moreover, the FE matrices' large condition-number, mainly caused by the inevitable high mesh graduation, requires special preconditioning techniques. The pre-conditioned conjugate gradient method (PCCG) is a well-established solver for FEM equation systems. A variety of CG-preconditioners has been developed and tested over the last years [10–15]. Addi-

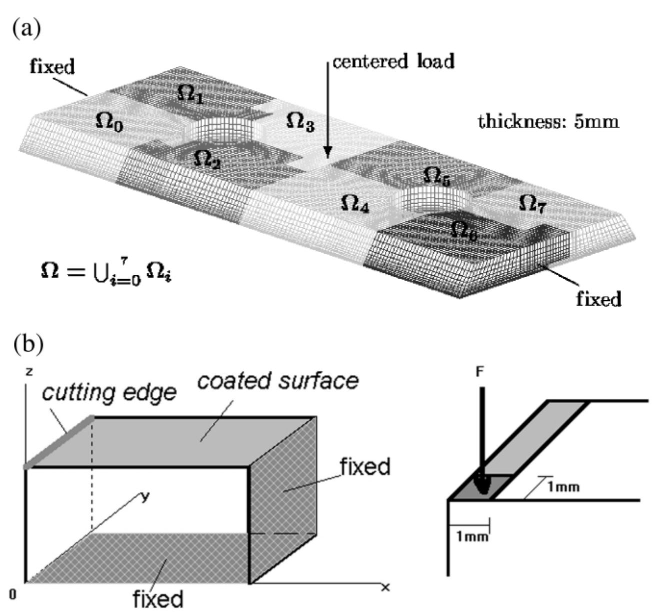

Fig. 1. Domain decomposition of a cutting insert with boundary conditions for a bending simulation (above) and boundary conditions for the simulation of a cutting situation (below).

tional coarse-mesh preconditioning has shown to substantially reduce the necessary number of iterations. For the presented simulations of coated tools, a PCCG solver with hierarchical BPX preconditioning [16] and an additional coarse-mesh solver was used.

4. Computational examples

Simulational results to the experimental oriented bending problem sketched in Fig. 1 have been published in [17]. A more application-related cutting situation will demonstrate the described method in this article:

A $12 \times 12 \times 5$-mm cutting insert made from metal carbide with $E = 600$ GPa is used for turning 34CrNiMo6 at a cutting speed of 250 m/min with width and depth of cut both being 1 mm. The calculated cutting force is $F = 3070$ N [18] and was assumed to act perpendicular to the chip-insert contact area (Fig. 1). The length of this contact area was assumed to be 1 mm. Using the force density function $f(x) = 6140(x-1)\mathrm{N/mm^2}$, which is constant in the y-direction and linearly decreasing in the x-direction, the cutting force is distributed over the contact area.

In addition to the geometry with clearance 0^0 (Fig. 1) the same technical process was studied for a cutting insert with a clearance of 11^0, distinguished in the sequel by the labels **Cl0** and **Cl11**. The stress analysis for this cutting situation was performed for the four layer systems shown and labelled in Fig. 2 with layer thickness 1.4 μm for MoST ($E = 147$ GPa), 2.4 μm for TiN ($E = 401$ GPa) and 3.0 μm for Al_2O_3 ($E = 360$ GPa). In the following, the notation ClxCoy with $x \in \{0;11\}$ and $y \in \{0;1;2;3\}$ denotes the simulational problem with clearance x and layer system y from Fig. 2. MoST is a special MoS_2 layer patented by Teer Coatings Ltd. Since the largest gradients of the solution are expected around the contact area, the grid lines in the x- and in the y-direction are concentrated and equally spaced in the contact area. Outside this region, the line distance was chosen to grow geometrically (Fig. 3). To reflect the thin coatings properly, the mesh in the layers is equally spaced, too, and in the substrate region the line distance in the z-direction grows geometrically with the distance from the coatings (Fig. 3). Fig. 4 shows the deformed mesh with node displacements magnified by 50. The clearance's influence on the tool's rigidity can be clearly seen, but in

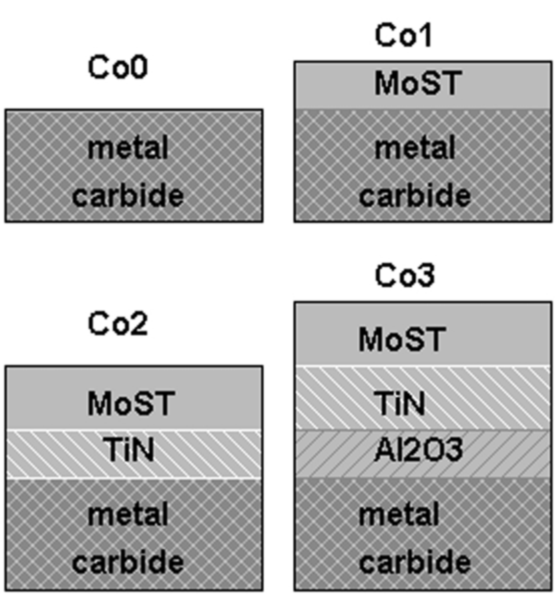

Fig. 2. Investigated coating–substrate systems.

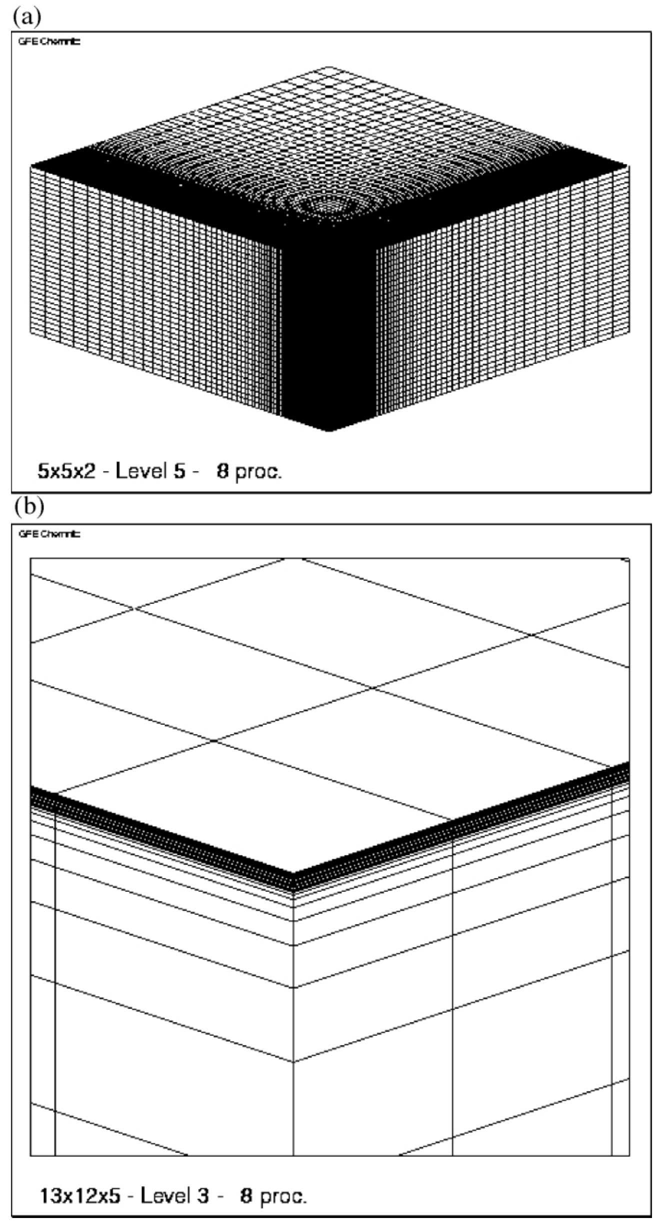

Fig. 3. Computational grid for **Cl0Co0** (above) and grid detail for **Cl0Co3** with 30 nm being smallest line distance (below).

Table 1
Computed displacement values

Scale unit μm	Cl0Co1		Cl11Co1	
	Min	Max	Min	Max
u_x	−6.4	0.27	−11.1	0.32
u_y	−5.0	0.19	−5.0	0.40
u_z	−17.5	0.00	−25.6	0.00

this coarse scale, the coating's influence is not detectable. The single components of the displacements varied as given in Table 1.

Both problems were simulated on a mesh comprising 855 393 nodes. The FEM assembly took 6.5 min. For the **Cl0Co1** problem, 2843 iterations/4.04 h were needed to solve the equation system, whereas the **Cl11Co1** problem took 3140 iterations/4.22 h. From the computed displacements, the equivalent stress and all the six stress components can be derived. The graphical presentations of the stress σ_{xx} in Fig. 5 and σ_{xy} in Fig. 6 clearly show the coatings' influence on the stress distribution. The brighter the colour in Figs. 5 and 6, the higher is the corresponding value. In Table 2 some numerical values are presented.

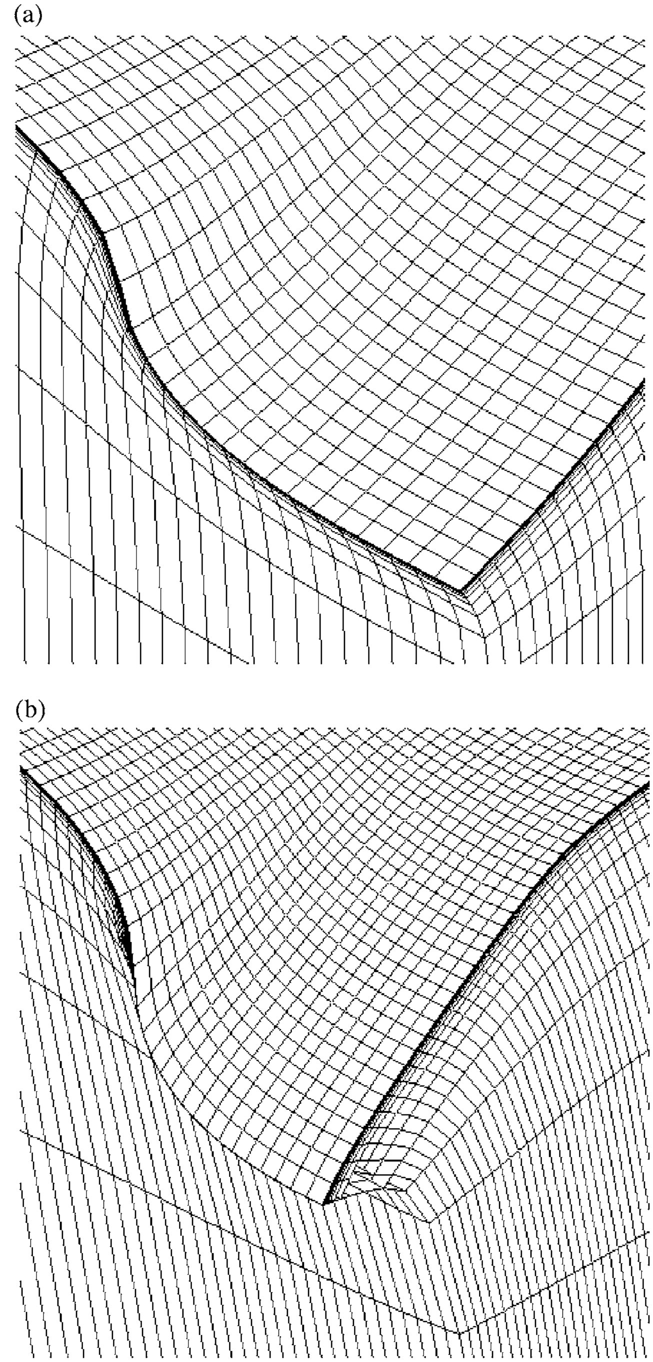

Fig. 4. Deformed meshes for **Cl0Co1** (above) and **Cl11Co1** (below).

5. Conclusions

Further progress in the design of new coating–substrate systems requires the combination of the still experimentally dominated developing process with numerical simulations on high resolution meshes for investigating the influence of external loads and heat sources on the coating stability. To overcome the long computational time for realistic three-dimensional simulations with a microscopic spatial resolution, parallel hardware should be used. Temperature distributions, deformations and stresses in coated cutting inserts caused by external loads can be computed by parallel FEM simulations with sufficient accuracy and detail resolution. This is possible for application oriented load situations as well as for experimental test situations. Computed results are available at the interior of the tool and in a surrounding of the material boundary layers, too. The presented method can contribute to a better understanding of the CSS's behaviour under specific load situations. It offers users of coated tools the possibility to judge the suitability of different coatings for their individual needs and manufacturers of coated tools a possibility to support the development of new coating systems by simulational computations. This way, the expense for the development of application-specific coating systems can be substantially reduced.

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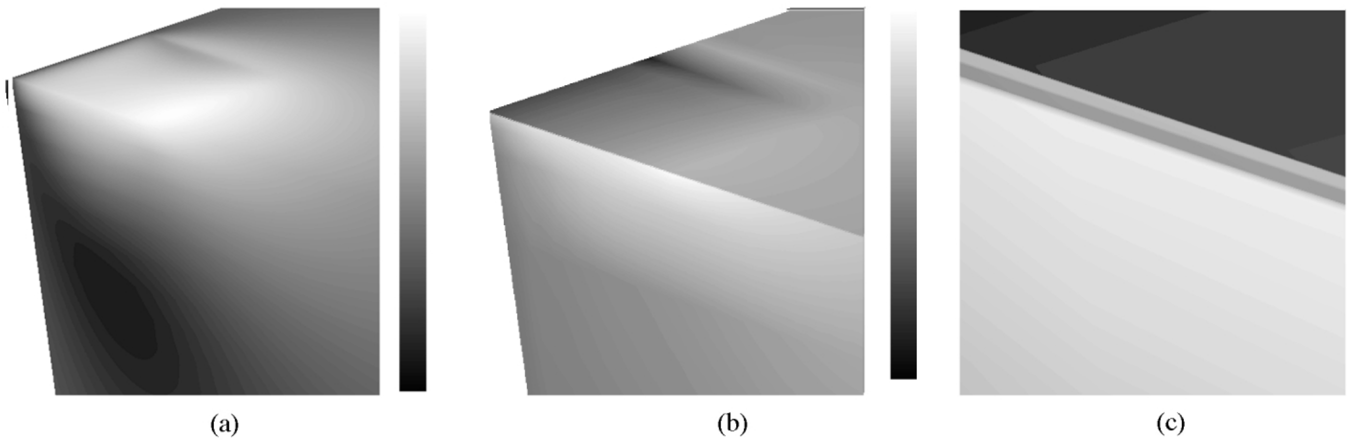

Fig. 5. Computed σ_{xx} for the problem **Cl11Co0** (left) and **Cl11Co3** (middle, right zoomed into the layer region).

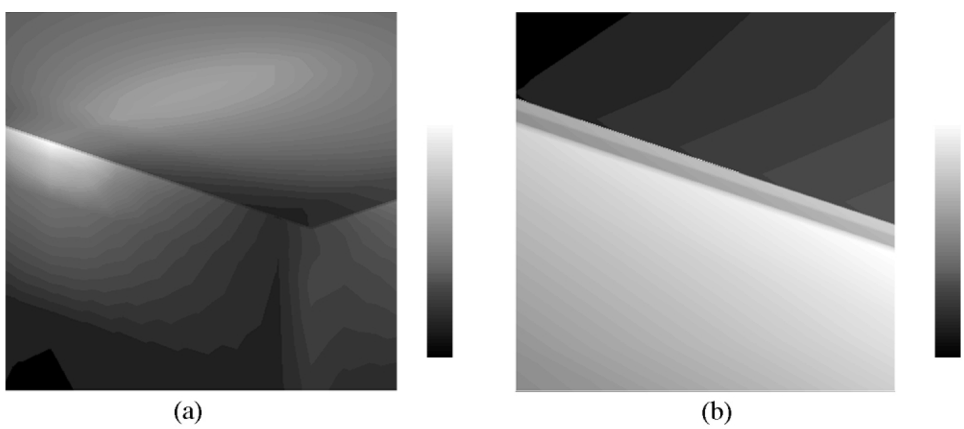

Fig. 6. Computed σ_{xy} for the problem **Cl0Co3**.

Table 2
Computed stress values

Scale unit MPa	σ_{xx}		σ_{yy}		σ_{zz}	
	Min	Max	Min	Max	Min	Max
Cl0Co0	−436	1890	−1700	1980	−6070	104
Cl0Co1	−1350	1910	−2200	2400	−6950	810
Cl0Co2	−1310	1920	−2040	2260	−6960	788
Cl0Co3	−1360	1620	−1910	1850	−6960	801

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