

# Deformation and fracture simulation of Ni<sub>3</sub>Al alloy under shock loads

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**Abstract.** A theoretical study of the deformation and fracture behavior of Ni<sub>3</sub>Al alloy under shock loading has been carried out. The finite element method simulation was used within the approach that combined modeling in terms of the dislocation kinetics of alloys with the L1<sub>2</sub> superstructure and the mechanics of a deformable solid. The dislocation kinetic model of the alloys with the L1<sub>2</sub> superstructure defined the hardening of Ni<sub>3</sub>Al punch and plate materials, while the model of the mechanics of a deformable solid described deformation of the macrovolume.

## 1 Introduction

Ni<sub>3</sub>Al intermetallide is related to the alloys possessing the L1<sub>2</sub> superstructure. Single crystals of these alloys are characterized by a temperature anomaly of mechanical properties. When heated, these materials become harder, and the yield stress increases. These alloys are widely used in high-temperature operation modes, including aviation and rocket technology. In particular, the Ni<sub>3</sub>Al intermetallic compound is used to manufacture the gas turbine engine blades.

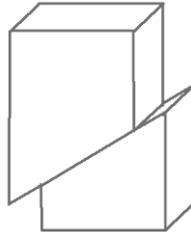
Despite the fact that these alloys demonstrate excellent performance in the high-temperature range, under uniaxial compression at the temperature  $T > 0.6T_{mp}$  ( $T_{mp}$  – melting point), a plastic strain superlocalization phenomenon [1, 2] was observed in single crystals of Ni<sub>3</sub>Al alloy as well as in Ni<sub>3</sub>Ge alloy that is isostructural to Ni<sub>3</sub>Al. The phenomenon is characterized by the formation of the bands of intense shearing, where practically all strain is concentrated, amounting to hundreds of percent. With that, the crystal regions remoted from the superlocalization band remain practically undeformed (Fig. 1). The phenomenon is similar to the formation of the adiabatic shear bands. The bands of superlocalization of plastic deformation as well as the adiabatic shear bands are formed upon significant heating of the material and are the result of phase transitions. For instance, the formation of the superlocalization bands in a single-crystal sample is accompanied by the formation of a polycrystalline structure in the band.

A model of the plastic strain superlocalization in single crystals of alloys with the L1<sub>2</sub> superstructure under uniaxial compression was proposed earlier in Refs. [3, 4]. Figure 2b presents the numerical simulation results. The model of this phenomenon was obtained due

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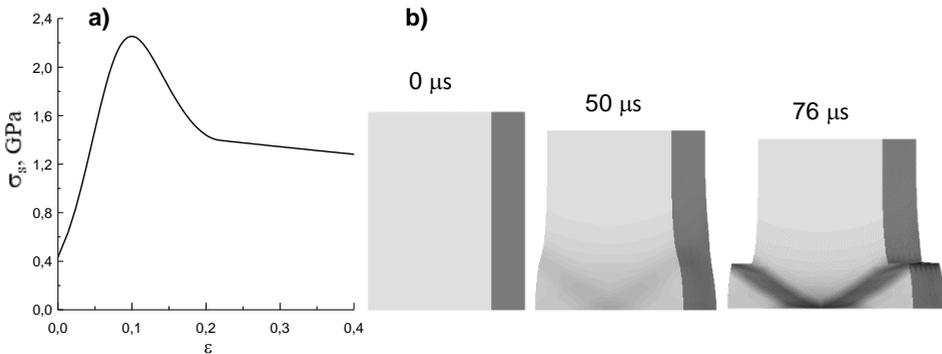
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to the approach that combines modeling in terms of continuum mechanics and dislocation kinetics of alloys with the  $L1_2$  superstructure. Thus, the dislocation kinetic model was used to set the properties of the material structure, and the mechanical model was used to describe the deformation of the macrovolume. Both experimental and theoretical studies of the reasons for the formation of the intense shearing bands were carried out in Refs. [3, 5,6].



**Fig. 1.** Schematic representation of localized shear.

Theoretical studies have shown that the required condition for the appearance of these bands in modeling is the setting of the hardening of the deformable material by a non-monotonic  $\sigma$ - $\varepsilon$  dependence (Fig. 2a) derived from the dislocation kinetics model. That is, not only should the hardening curve of the material possess a section characterizing its hardening, but also a section corresponding to its softening, e.g., due to the structural transformations.



**Fig. 2.** a)  $\sigma$ - $\varepsilon$  dependence defining material hardening, b) distribution of the plastic strain intensity values at different times of sample deformation.

The present work aimed to reveal the effect of the nature of hardening of the  $Ni_3Al$ -based plate and punch materials, defined by the model of dislocation kinetics, on the deformation and fracture behavior during the shock punch-plate interaction.

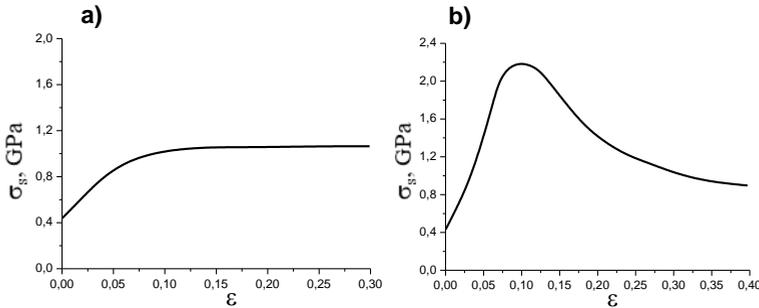
## 2 Methods

The calculation of the shock interaction plate and punch were carried out using the approach that combines modeling in terms of continuum mechanics and dislocation kinetics of alloys with the  $L1_2$  superstructure. The model of the dislocation kinetics of the alloys with the  $L1_2$  superstructure, based on the storage-recovery framework, is described in details in Refs. [3, 4].

The model of the mechanics of an elastoplastic medium describes the deformation of a macrovolume represented as a matrix material with inclusions of voids. The system of equations describing the motion of a void elastoplastic medium includes the mass,

momentum, and energy conservation laws, constitutive equations of the plastic flow theory and the equation of state in the Mie–Grüneisen form. The local criterion for the split fracture is the critical value of the relative void volume. The critical value of the intensity of plastic deformation is considered a local criterion for shear fracture. A detailed description of the mechanics model and the method to combine these models are given in Refs. [3, 7]. The combined model is implemented in the “RANET-3” software complex [8] that allows solving problems in a full three-dimensional formulation using the finite element method (FEM) modified to solve the dynamic problems.

The  $\sigma$ – $\varepsilon$  dependences (Fig. 3) characterizing the hardening of the Ni<sub>3</sub>Al alloy were obtained by varying the parameters of the dislocation kinetics model to control the redistribution of dislocations into the dislocation walls.



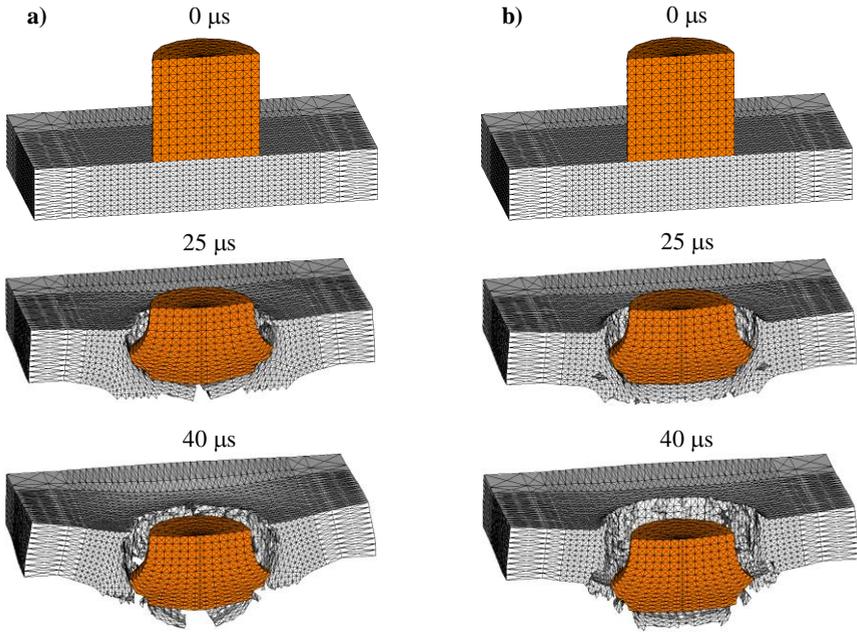
**Fig. 3.** Stress-strain curve of Ni<sub>3</sub>Al alloy obtained by solving the equations of the dislocation kinetics model for alloys with the L1<sub>2</sub> superstructure.

The calculations of the Ni<sub>3</sub>Al plate deformation under shock loads with steel punch was carried out. The parameters of the calculations were as follows: plate thickness was 10 mm, the height and the diameter of the punch were 20 mm, the initial punch speed was 900 m/s.

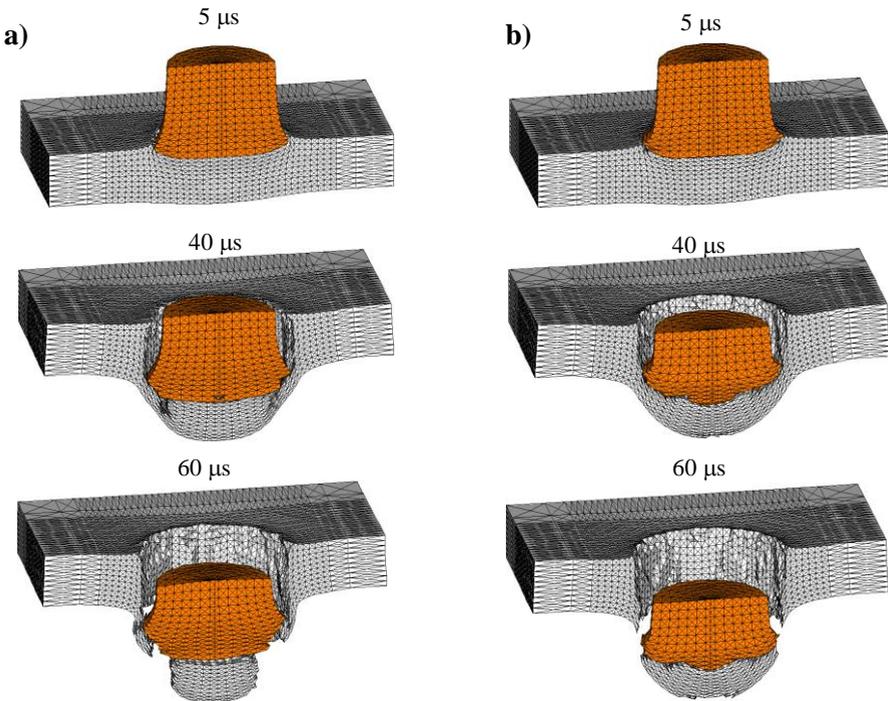
### 3 Results

Figure 4a presents the FEM-based simulation of the interaction of the Ni<sub>3</sub>Al plate with steel punch, when the plate hardening is defined by the monotonic stress-strain curve (Fig. 3a). In the initial time of interaction, a fracture occurs by a split mechanism on the back surface of the plate as a result of the interaction between the internal shock release waves that propagate from free surfaces of the plate and the punch. At 25  $\mu$ s, the spreading split fracture reaches the point of contact with the punch. At 40  $\mu$ s, the plate is punched. The punch speed behind the plate is 426 m/s.

The split fracture is less intensively propagated on the back surface of the plate in the initial moments of the interaction (Fig. 4b) than with the monotonic hardening curve (Fig. 4a), if the hardening of the plate material is defined by the non-monotonic stress-strain curve (Fig. 3b). This may be due to the more intense initial stage of stress growth with increasing strain on the non-monotonic hardening curve (Fig. 3b). In this case, two small split fractures are also formed on the sides of the point of contact with the punch. The split fractures then propagate to the crater surface. The punch speed behind the plate is 429 m/s. The passing of the punch through the plate occurs more intensively than with a monotonically increasing hardening curve. Probably, this is due to the formation of the intense shearing bands at the crater edges during the passing of the punch. The formation of more even crater edges (Fig. 4b) than in the previous case (Fig. 4a) may also indicate this.



**Fig. 4.** FEM-based simulation results of interaction of the  $\text{Ni}_3\text{Al}$  plate with the steel punch, when the hardening of the  $\text{Ni}_3\text{Al}$  alloy is defined by a) monotonically increasing  $\sigma$ - $\epsilon$  dependence, b) non-monotonic  $\sigma$ - $\epsilon$  dependence.



**Fig. 5.** FEM-based simulation results of interaction of the  $\text{Ni}_3\text{Al}$  punch with the steel plate, when the hardening of the  $\text{Ni}_3\text{Al}$  alloy is defined by a) monotonically increasing  $\sigma$ - $\epsilon$  dependence, b) non-monotonic  $\sigma$ - $\epsilon$  dependence.

The next series of calculations were performed to study the deformation behavior of the Ni<sub>3</sub>Al punch interacting with a steel plate. The hardening curves for the punch material were set the same as for the previous calculations. Figure 5a presents the FEM-based results of the interaction of Ni<sub>3</sub>Al punch and steel plate when the hardening of the punch material is defined by the monotonic stress-strain curve (Fig. 3a). In this case, the punch is broadened in the site of interaction with the plate. The fracture occurs by the shear mechanism at the edges of the punch during its further passing through the plate. The punching of the plate occurs at 60  $\mu$ s. The punch speed behind the plate is 258 m/s.

If the hardening of the punch material is defined by the non-monotonic stress-strain curve (Fig. 3b), the formation of a pointed area of the punch can be observed (Fig. 5b) during the passing of the punch through the plate. This may indicate the beginning of the formation of the adiabatic shear bands resulting in self-sharpening of the punch. This may increase the ballistic efficiency. The punch wears more than in the previous case. The punching of the plate occurs at 55  $\mu$ s. The punch speed behind the plate is 293 m/s.

## 4 Conclusion

Thus, the type of  $\sigma$ - $\varepsilon$  dependence, setting the hardening of the plate and punch materials, has a significant impact on the processes of deformation and fracture during their high-speed interaction. The setting of hardening of the Ni<sub>3</sub>Al plate material in the form of a non-monotonic  $\sigma$ - $\varepsilon$  dependence probably leads to the formation of the adiabatic shear bands during the high-speed interactions with a steel punch. The punching of the plate proceeds more intensively, if the hardening is defined with a non-monotonic curve, than in case of the monotonic  $\sigma$ - $\varepsilon$  dependence that does not envisage the softening of the plate material.

Setting the hardening of the Ni<sub>3</sub>Al-based punch material in the form of a non-monotonic dependence may also lead to the formation of adiabatic shear bands during the high-speed interactions with a steel plate. As a result, the effect of self-sharpening of the punch material takes place increasing its ballistic efficiency.

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