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Computer Applications in Metallurgical Research

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ABSTRACT

This paper outlines the current efforts in computer applications in metallurgical research at the Defence Metallurgical Research Laboratory, Hyderabad. Work being done on armour penetration studies, optimization of armour profiles for fighting vehicles, computer control of multifunction 2000 tonne forge press, drawing of processing mechanism maps, process modelling of titanium sponge production and methods of curve fitting to experimental data, is described and briefly discussed.

1. INTRODUCTION

Metallurgical research is largely based on experiments. It derives support from thermodynamics, kinetics, and composition-microstructure-property correlations. It is also dependent on many qualitative and semi-quantitative analyses and ideas based on similarities and similitudes. Metallurgical research usually defies analytical approaches. Nevertheless, computers are now becoming extremely useful in many ways. They are being used to control equipment and processes, to record and analyze data. We are now able to generate nearly quantitative solutions through careful computer simulations thereby substituting costly experiments. Computer simulation promises to save enormous time, effort, and money, thereby accelerating the pace of metallurgical research.

In this paper we discuss a few recent examples of computer applications in metallurgical research at Defence Metallurgical Research Laboratory (DMRL), Hyderabad.

2. MODELLING OF THE RESPONSE OF ARMOUR MATERIALS

Penetration of metal targets by projectiles is influenced by many parameters such as material properties, impact velocities, projectile shape, target support, relative dimensions of target and projectile. For a thorough understanding of penetration process, it is necessary to identify the important material properties and to know how they relate to the failure of the target. Computer codes are useful in such investigations.

2.1 Numerical Model

At DMRL, a computer code named PRHD, has been successfully employed to model the penetration process. This code is a 2-dimensional, multimaterial, Lagrangian code for solving material flow problems in the hydrodynamic and elastic-plastic regimes. The material model employed in PRHD includes an equation of state, such as Tillotson equation of state, a deviatoric constitutive relation for elastic and plastic deformation, and a failure criterion such as the Von Mises yield criterion.

If v_i is the impact velocity and v_s is velocity of sound in material, then for $v_i < v_s$ the Tillotson[1] equation of state has the form

$$P = A.\mu + B.\mu^2 \tag{1}$$

and for $v_i > v_s$

$$P = A.\mu + B.\mu^2 + [A.\mu e^{-B(v^{n-1})}].e^{-a(v^{(n-1)^2})} \tag{2}$$

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where, $\mu = 1/V-1$ and V = relative volume.

In Eqns (1) and (2), $A, B, \mu, ß, \alpha, n$ are constants for the particular material. The Von Mises yield criterion can be written as

$$\sigma_{eq} = \sqrt{3/2} \, . \, \sqrt{2J} \tag{3}$$

where $2J = s_{xx}^2 + s_{yy}^2 + s_{\theta\theta}^2 + 2T_{xy}^2$ (4)

A variable yield strength (Y) in shear can be of the form

$$Y = Y^{\circ}.(1 + \varepsilon_{eq})^n \tag{5}$$

with

$$\varepsilon_{eq} = \varepsilon_{00} + \varepsilon_{01}.X + \varepsilon_{02}.X^2 + \varepsilon_{03}.X^3 + \varepsilon_{04}.X^4 \tag{6}$$

where $X = 1-V$

Table 1 indicates the typical values of the constants used in the model.

Table 1. Constants of the numerical model

Parameter	Unit	*Al*	Mild steel	*Cu*	*W*
A	Mbar	0.7520	1.2800	1.3900	3.0800
B	Mbar	0.6500	1.0500	1.1000	2.5000
α		5.0000	5.0000	5.0000	10.0000
ß		5.0000	5.0000	5.0000	10.0000
Y°	Mbar	0.0029	0.0034	0.0012	0.0220
ρ	g/cc	2.7000	7.8600	8.9000	19.1700
γ		125.0000	40.0000	36.0000	77.0000
n		0.1000	0.3500	0.4500	0.1300
ε_{00}		-0.0028	-0.0013	-0.0012	-0.0004
ε_{01}		-0.0056	-0.0029	-0.0023	-0.0006
ε_{02}		0.1364	0.1012	0.0753	0.0306
ε_{03}		0.2495	0.2051	0.1526	0.1336
ε_{04}		0.3160	0.2901	0.2190	0.1604

2.2 Example

Figure 1 shows the projectile-target configurations at various times for a 6 mm diameter steel conical

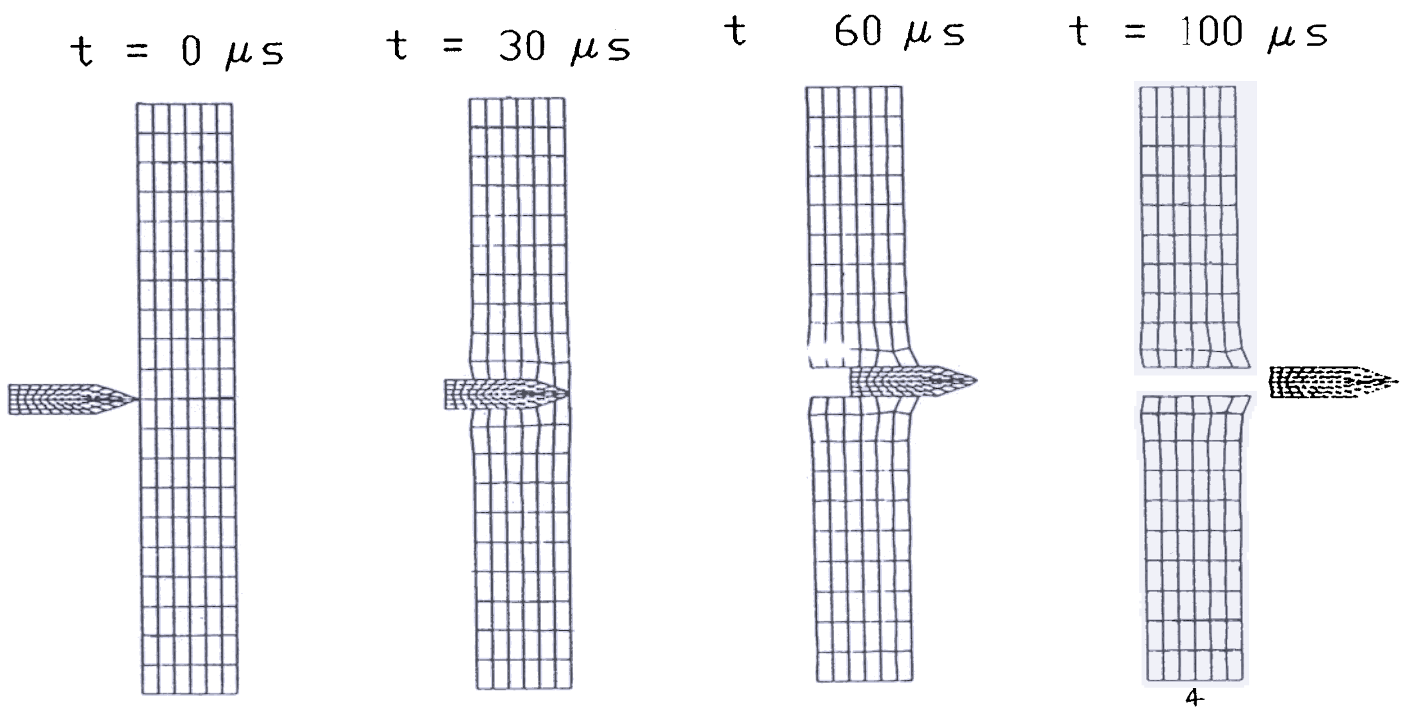


Figure 1 Simulation of penetration at different time steps.

projectile of L/D ratio of 4.5 impacting a 20 mm thick mild steel plate at a velocity of 800 m/s. The complete perforation takes place in 90 μs.

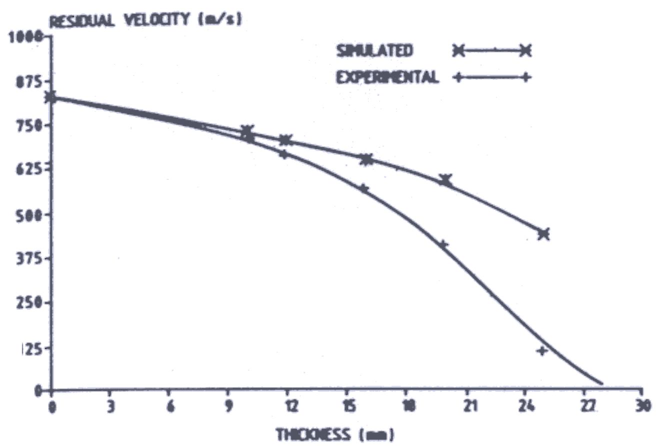


Figure 2. Simulated and experimental results of residual velocity.

Figure 2 shows typical experimental results along with the results of computer simulation. It may be seen that the results of computer simulation match the experimental results reasonably well.

3. OPTIMIZATION OF THE ARMOUR PROFILE FOR VEHICLES

Design of the armour profile for parts of vehicles such as a turret for any battle tank is complicated by the constraints posed by the overall design specifications for the battle tank. For example, in the battle tank the gun control system, turret traversing system and other limitations have to be taken into account to optimize the weight and dimensional penalties of the armour on the turret and thereby increase the protection level of the tank against different anti-tank ammunitions.

We have developed a mathematical model of the turret to simulate the various turret functions such as rotation. The package is modular and works in two phases : a mathematical phase and a graphics phase. The mathematical phase views a turret basically as a shape developed with various intersecting plates. The profile consisting of inner surface of these plates is referred to as 'inner profile' and that of the outer surface as the 'outer profile'. The armour lies within these 'inner' and 'outer' profiles. For each plate, the structure and thickness of composite armour is decided depending on the angle of attack and the type of ammunition. The outer profile can be obtained by adding these thicknesses to the corresponding surfaces of the inner profile. The weight and location of centre of gravity of each plate are computed next. These data are then combined with the other data of the tank to determine the overall weight and out of balance moment. Different profiles are analyzed to select the one which offers the best possible protection with the least weight and dimensional penalties.

The graphics phase of the software facilitates the viewing of the designed turret profile. It also permits turret rotation and allows us to check the design flaws, interferences and constraints.

Figure 3 shows an example of optimized turret profile at two different positions. The limitations at the driver's hatch in some positions can be seen clearly.

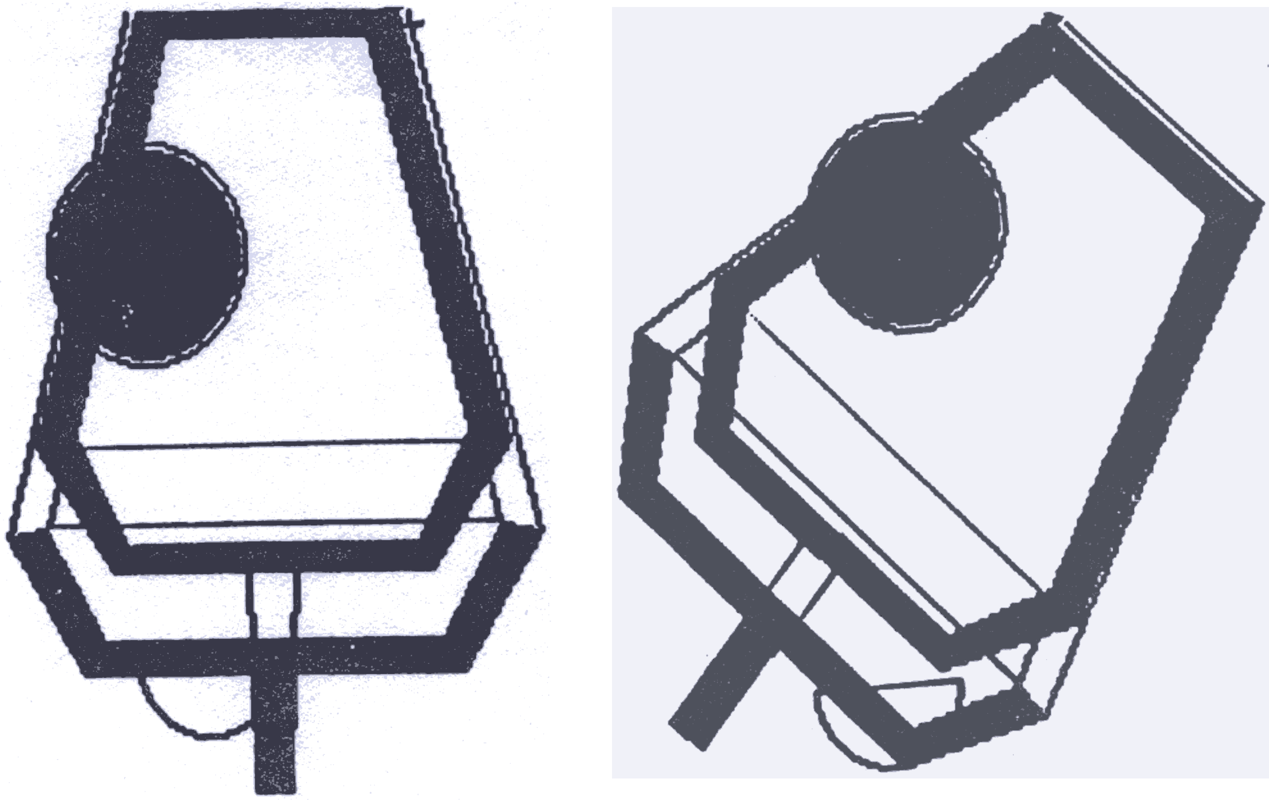
4. COMPUTER CONTROL OF MULTIFUNCTION FORGE PRESS

Forging is one of the oldest methods of hot metal forming. Essentially it consists of applying a controlled amount of force on a hot metal. Though the principle of forging operation is simple, there are a number of variations in modern forging operations : open die forging, closed die forging, isothermal forging and liquid metal forging. In industrial practice, separate equipment are used to carry out each of the above mentioned forging operations.

The advent of microprocessor technology in the seventies has made it possible to integrate the above functions into a single equipment, thus substantially reducing the capital investment.

At DMRL, hot metal forming technologies are being developed for aluminium, titanium and other materials for defence applications on a 2000 tonne multifunction forge press. This press is unique in that it incorporates all the modes of forging. It also provides a capability for metal extrusion.

The forge press is hydraulically operated and controlled by a state-of-the-art electronic control system. The block diagram of the system is shown in Figs 4 and 5. The control system is built around 8-bit, Z-80 microprocessors in a modular fashion. The motor-control-centre (MCC) which controls the different electric motors driving the hydraulic pumps is monitored and controlled by the 'Electric Control Processing Unit (CPU)'. A number of digital input/output channels are



PLAN VIEW (ΦDEG ROTATION)   PLAN VIEW 45DEG ROTATION)

Figure 3. Turrent profile rotation.

provided to start/stop motors and to monitor alarm conditions area such as motor, electric, or thermal overloads. The 'Press CPU' controls and monitors the press movement, speed, force and position. The 'Manipulator CPU' controls and monitors the manipulator travel, jaw movement, clamping force, and integrates the movement of the manipulator with the press strokes. The 'data record CPU' logs various parameters like press-force, position, speed, column-stretch, die-temperature and piece-temperature while the forging operation is in progress. Each of the above processors are loosely coupled and exchange messages over serial links. The control system further provides for equipment diagnostics and safety interlocks.

A supervisory computer (Fig. 4) in the form of an IBM PC/AT is provided to down-load forge programmes on to the control system in the 'CNC' mode of operation of the equipment. Further, in the 'copy' mode of operation it is possible to carry out a sequence of forging steps manually on a job and have these steps copied on the supervisory computer. Later, the steps can be 'replayed' on a similar job.

One of the major features of this press is the provision for data collection. Temperatures, positions, speed and strains at different locations are monitored throughout the operation of the press. Computer control is used to advantage in recording these data continuously on the PC. The data can be later recalled for detailed analysis.

Using the computer interfacing and data acquisition facility of the forge press, parameters for open die forging of titanium alloys and extrusion of advanced aluminium alloys have been established. As an illustration, a plot of forging force versus displacement during the near isothermal forging of IMI-685 material is shown in Fig. 6. Such data are useful for detailed studies on processing of various materials.

5. PROCESSING MAPS

Deformation processing of materials requires the selection of the correct process parameters, viz. temperature and strain rate, so as to increase the yield and improve the quality of the product. Trial and error methods generally employed for optimizing these

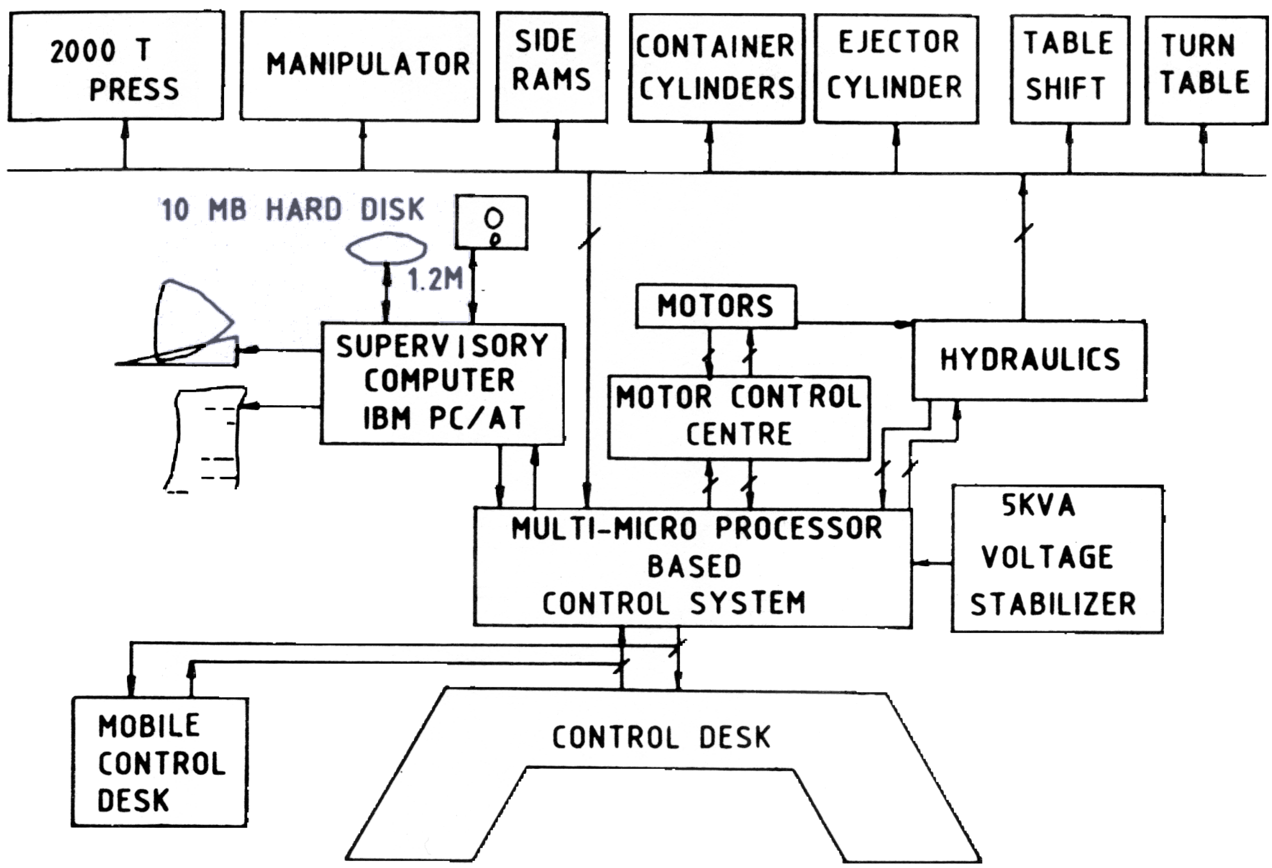


Figure 4. Block diagram of 2000 *T* forge press.

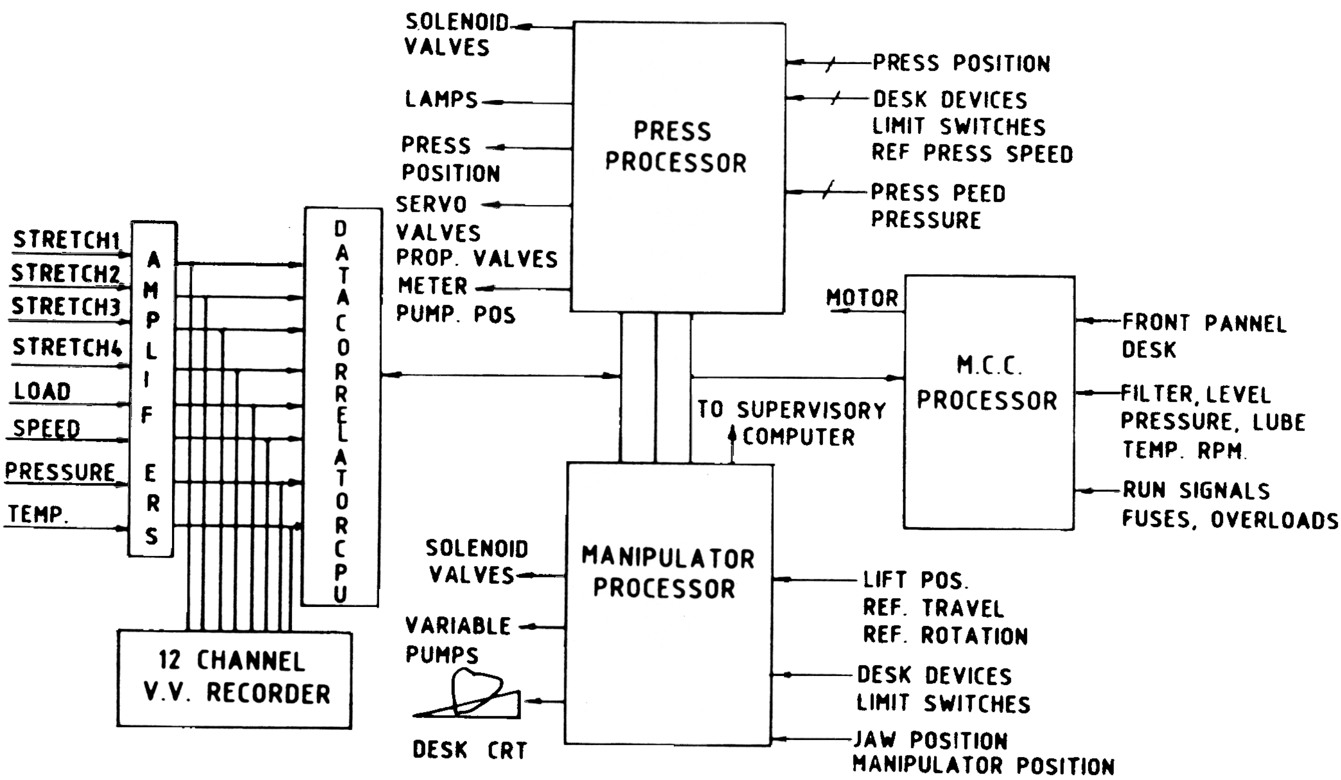


Figure 5. Block diagram of forge press control system.

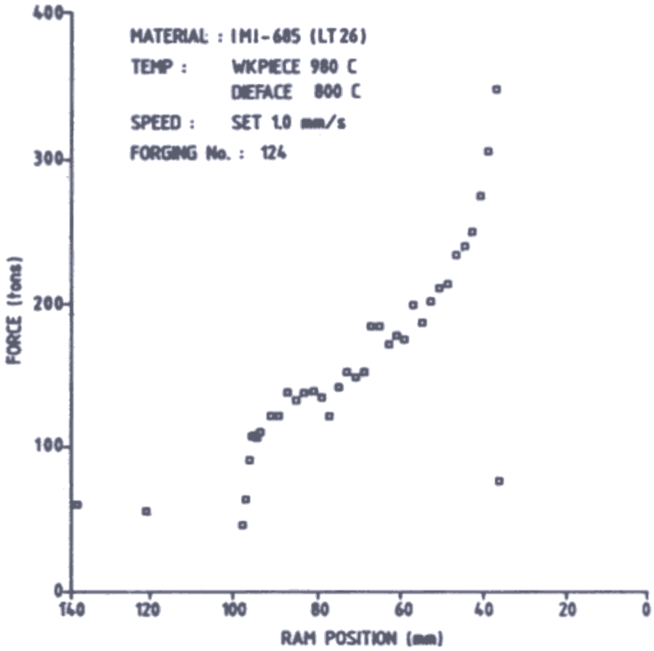


Figure 6. Plot of forging force vs displacement.

process parameters are both costly and time consuming. Further, the conventional methods become too difficult for optimizing the process parameters of advanced materials such as intermetallics or metal-matrix composites. Processing maps depicting the variation of the efficiency of power dissipation on a strain rate versus temperature domain, provide an alternative method of identifying safe processing zones as well as optimum processing parameters. This method, based on laboratory scale experiments, has also the advantage of being quick, economical, convenient and reliable.

The concepts of processing maps developed by Prasad *et al*[4] is based on a dynamic material model. It follows the physical systems-modelling approach. Deformation modelling is considered as a system in which the workpiece material is a dissipator of power. The power input into the system is assumed to be dissipated in the form of dynamic microstructural processes and the viscoplastic heat. Partitioning of power between these two is related to the strain rate sensitivity of the material. Hence, the efficiency of the power dissipation through microstructural processes is given as a function of the strain rate sensitivity and, for a given workpiece material, the efficiency serves as an index of dynamic material behaviour. The processing map[5] shown on Fig. 7 represents constant efficiency contours in a strain rate versus temperature domain. It has been interpreted to show regimes where processes such as dynamic recovery, dynamic recrystallization, void formation and wedge cracking dominate.

These maps can be easily constructed with the help of a computer software[6] mentioned above. The data input for the software is obtained from simple hot compression tests on laboratory scale specimens of the material. We thus have a simple and powerful tool for optimizing the processing conditions of all materials.

6. PROCESS MODELLING FOR TITANIUM SPONGE PRODUCTION

Titanium metal is industrially produced by reducing $TiCl_4$ with liquid magnesium or sodium in steel reactors under argon atmosphere. The reduction reaction is exothermic. The process is generally managed by controlling the process parameters like feed rate of $TiCl_4$, reaction temperature and external cooling of the reactor. Computer-based control for sodium reduction process is adopted. A statistical control strategy is normally adopted for magnesiothermic reduction process because satisfactory models for the reaction mechanisms are not available.

In the present study at DMRL, an attempt has been made to develop a reaction model for its use in the process control. As a first step, computer-based calculations were made for prediction of temperature distribution inside the reactor using finite element method. The temperature data were utilized to calculate the reaction rate constants affecting the rate of the overall reaction.

The reaction kinetics is assumed to be determined by a combination of intrinsic reaction rate-determining factors and also the sponge growth rate kinetics involving the following steps :

(a) convective mass transfer of titanium tetrachloride to the reaction front (*Kg*)

(b) the surface chemical reaction (*Ks*)

(c) exchange of reactants through the porous solid barrier (over the liquid magnesium) (*Ke*).

6.1 Temperature Profiles

The heat generated in the reduction reactions is transferred to the reactor walls by conduction through the reaction mass. A knowledge of temperature distribution inside the reactor is essential for determining the reaction rate constants.

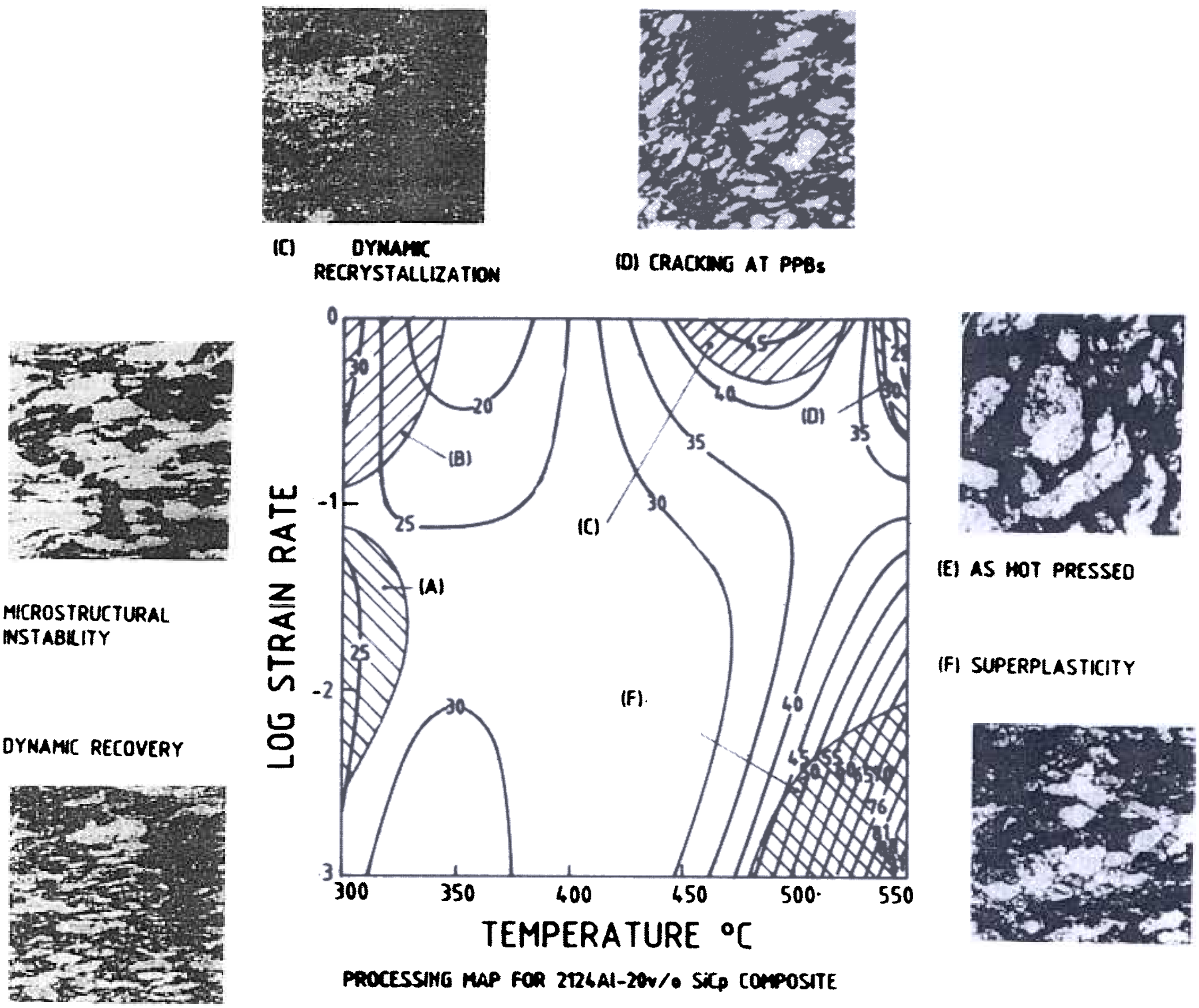


Figure 7. Processing map for 2124 *Al*- 20v/o *SiCp* composite.

The governing differential equation for heat conduction in an axisymmetric cylindrical body is

$$K\left[\frac{\delta^2 T}{\delta r^2} + \frac{\delta T}{r\,\delta r} + \frac{\delta^2 T}{\delta z^2}\right] \qquad \frac{\delta T}{\delta t} \qquad (7)$$

This was solved by the finite element method with the following initial boundary conditions :

$t = 0,\quad T = 830$ °C throughout the mass
$t > 0,\quad T = 860$ °C at the walls

and

$$K\left[\frac{\delta T}{\delta r}\, l_r + \frac{\delta T}{\delta z}\, l_z\right] + h\ (T - T_\infty) = 0 \qquad (8)$$

A program has been developed in FORTRAN to solve the above equation and it was run using DPS-6/850 super mini computer for various $TiCl_4$ feed rates. Figure 8 shows the surface temperature profiles computed for different $TiCl_4$ feed rates.

6.2 Kinetics Modelling

The reaction rate constants of the three steps, *Kg*, *Ks* and *Ke* were determined using the physicochemical data available in the literature. The temperature data required for these calculations were taken from the results of the program.

The overall reaction rate constant, *Ko*, is determined as,

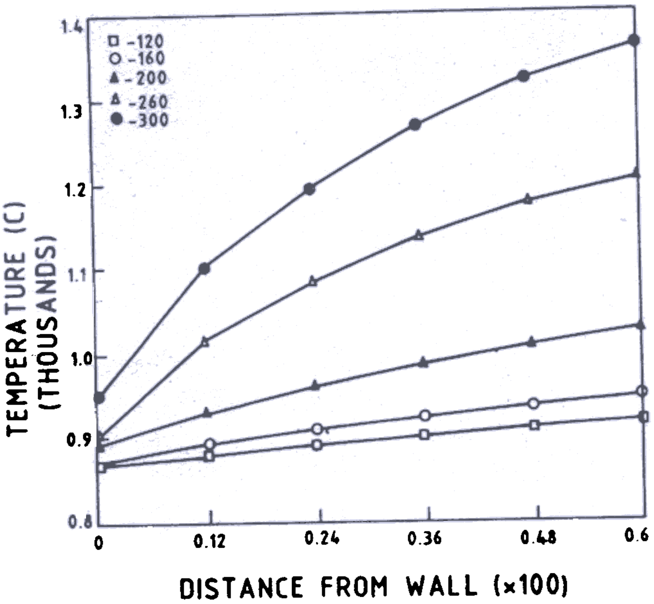


Figure 8. Temperature profiles.

$$\frac{1}{Ko} = \frac{1}{Kg} + \frac{1}{Ks} + \frac{1}{Ke} \qquad (9)$$

The experimental conversion rate constant (Kr) is found to be related to the overall reaction rate constant by,

$$Kr = K_o^2/h_o$$

The rate of conversion of magnesium is given as

$$-\ln(1-X) = 497.2\frac{Kr}{h_o}.t^2 \qquad (10)$$

where t is time in seconds and h_o is the height of the initial magnesium column in the reactor. This expression is found to be valid for nearly 70 per cent conversion of magnesium.

7. CURVE FITTING

A simple yet immensely useful area where the digital computer contributes in engineering applications is that of curve fitting. We have developed a package in FORTRAN that can be used for polynomial regression curve fitting as well as adaptive piece-wise curve fitting.

For polynomial regression curve fitting, the well known least-squares method is used. In the program, either the degree of approximating polynomial may be specified or the best-fit polynomial can be obtained.

For adaptive piece-wise curve fitting, two methods called l^1 sense and l^2 sense are employed. The l^1 sense is similar to the simplex method of linear programming and the l^2 sense employs the Householder transformations. It is best to use the l^1 sense for data containing noise, especially when the data are large.

The piece-wise curve fitting part of the package is completely adaptive in nature and is different from the traditional curve fitting methods. Whereas the traditional methods require the total number and locations of knots to be specified in advance, the present package calculates by itself the total number and location of knots needed.

The inputs for this package are: X-Y coordinates degree of approximating polynomial number of continuous derivatives, and error tolerance.

At DMRL this package is being used for many curve fitting applications to fit the experimental data.

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