

# Analysis of Kinetic Energy Effect in Molecular Deformation of Aluminum 6063 Alloy

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**Abstract:** The matrix repatterning process during the cause of molecular deformation is studied. Aluminum 6063 alloy, which was melted at 650°C and subjected to two solidification kinetics, (vibratory and static), in a steel die mould. The evaluation of molecular parameters, the velocity, pressure, and temperature of the alloy were obtained during the experimental process to assess parametric properties and influence on the molecules as deformation occurred. It was revealed that velocity of impact dominates the experimental temperatures and pressures recorded. Moreover, vibrated solidification process possessed more impact absorbing energy than static cooling process. Conclusively, the evaluations of the most probable speed show that temperature for static cooling was reached faster than that of vibrated solidifications. Thus, kinetic energy had great effect in delocalization and deformation process of molecules of the material.

**Index Terms:** Aluminum 6063 alloy, Kinetic Energy, Velocity, Molecular distribution, deformation, vibratory and static process.

## 1. Introductions

The reactions of materials to an applied load depend on the modes of its applications; various research studies brought up the fact that force of impact on material molecule culminates in the transition from kinetic energy, through potential energy then back to kinetic or heat energy [1],[2],[3],[4].

When a material in stationery position is hits by certain load the motion of such load influences the motion of free electron molecules in material [5]. These excited molecules occupying the next available vacant position, hence resulting into deformation in a macro scale. [6]. The kinetic energy therefore is absorbed by the movement of the electrons and a great amount of heat is released hence causing their forces to be neutralised. [6].

According to [7], who examined the effects of tensile deformation rates on tensile properties of polypropylene, affirmed that deformation parameters had great influence in the deformation of the material but in their analysis tensile rate of deformations was evaluated leaving out the internal effect of mechanism that brought about the process and ultimate tensile properties of the material. The elastomeric network deformation analysis of molecular and classical statistical model of elastic

deformation by [8] further analysed the detail insight into the initial molecular network structure as well as the evolution of the network with deformation and the resulting stress-strain behavior of the materials. In addition, the evolution of uniaxial deformation using molecular dynamics techniques to explain the behaviour of glassy polymers was studied by [9]. Furthermore, Cold Gas Dynamic Manufacturing that uses a surface coating technique in a supersonic gas jet employs the high kinetic energy of the particles to effect bonding through plastic deformation upon impact. Although the researches gave rise to formation of the prototype required, but the study devoid of individual effect of determined parameters (especially the mass flow rate and transfer speed of the molecule). Hence, the structural presence of oxygen across interfacial boundaries was a great concern, [10]. Moreover, the molecular dynamics of materials have always been worked on and centered basically on diffusion and concentration of the molecules in reference to temperature and pressure propagations [11],[12]. Nevertheless, dynamic delamination and mass loss of composite material that gave way for kinetic energy evaluation was analysed by [13]. From the observation by various fundamental researches, the validity of solidification theories, in particular for the rapid solidification process under highly super-cooled conditions, largely depends on the accuracy of thermophysical data. [14],[15],[16] and [17]Zhang et al, (1991); Takeuchi and Inoue, (2000); Johnson, (1999) and Bormann, (1994). The simulation of solidification process by [18] Bodner, S. R. (1968) explained vital parameters of

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the solidifications a number of these crucial parameters were therefore evaluated in their studies. But the study was unable to relate the individual effect of the velocity, kinetic energy, temperature and pressure during the deformation process. For the reasons that, molecular transformation in material during the cause of plastic deformation, distortion and dislocation of molecules require more understanding, the analysis of its matrix repatterning is going to be performed in this study.

## 2.0 Materials and Methods

### 2.1 Experimental Procedures

Aluminum alloy of Al – Mg – Si type was cast in a pre heated steel mould. This was done on two different surfaces: a static (on a bare floor) and a vibrating surface (with the use of a vibrator). Heating the ingot to 663°C, casts on the static surface was achieved by pouring the stirred molten charge in the cylindrical mould cavity of the die which was placed on a cemented floor. As regards the vibrating surface, the melt was poured into the die cavity placed on a vibrator operating at 0.5Hz. After twenty seconds, the die with its content were made to cool to ambient temperature. The cast samples were ejected from the die after solidification by unlocking the mould and for each casting a 40mm diameter and 140mm high cylindrical sample was achieved. Four castings, one for each reduction via deformation were carried out on both static and vibrating floors respectively.

The effect of kinetic motion of the particle on temperature and its subsequent contribution to pressure in the molecular deformation of particle is analysed using momentum and Newton’s law of motion.

For the kinetic effects, using the knowledge of average velocity of the system obtained during the experimental process, the temperature variations of the system were evaluated as follows [19](Fitzpatrick 2012):

$$\frac{1}{2} m \overline{v^2} = \frac{3}{2} k_B T \tag{1}$$

$$T = \frac{m \overline{v^2}}{3k_B} \tag{2}$$

M=mass;  $k_B$ = Boltzmann constant;  $v$ = Average velocity;  $T$ = Temperature.

Assuming an elastic collision of the hammer with the wall of the materials, the pressure distribution causes a great influence in the molecular number per unit volume

disturbance in the system. Hence, pressure is proportional to the number of molecules per unit volume ( $N/V$ ) and to the average translational kinetic energy of the molecules and is therefore expressed as [20]Kittel, (1979);

$$P = \frac{2}{3} \left( \frac{N}{V} \right) \left( \frac{1}{2} m \overline{v^2} \right) \tag{3}$$

$$K.E = \frac{3}{2} N k_B T \tag{4}$$

$$N = \frac{2 K.E}{3 k_B T} = \frac{3 k_B P V}{m \overline{v^2}} \tag{5}$$

$N$ = number of molecule,  $K.E$ = Kinetic energy;  $P$ = pressure distributions

The kinetic energy pressure distribution and number of molecule per unit volume is thus related as shown above.

Furthermore, using the knowledge of equi-partitioning of energy in complex molecules, other contributions to internal energy must be taken into considerations. One possible energy source as related to this experiment is the translation motion of the center of mass and another is vibration motion. Both potential and kinetic energy are associative with this motion causing effects and displacement in their internal energy to allow for possible distributions. When this occurred the internal energy of the system is expressed as [20]Kittel, (1979):

$$E_{INT} = \frac{7}{2} n R T \tag{6}$$

$E_{int}$ =Internal energy of the system;  $n$ = mole fraction  $R$ = Gas constant;

The internal energy, number of molecule per unit volume and the temperature in the system is related by Boltzmann distribution law as expressed in[20] Kittel, (1979).

$$n_v(E) = n_0 e^{-E/(k_B T)} \tag{7}$$

$n_v$ = number of molecule per unit volume,  $n_0$ = initial mole fraction of the material and

$E$ = energy generation

In quantization mechanics, energy is proportional to the frequency of the wave, therefore, the number of atoms and molecules are quantized.

Although rotation and vibration are classically allowed, they do not occur because as the temperature increases, the energy of the molecules increases. In some collisions,

the molecules have enough energy to excite to the first excited state; thus as the temperature increase, more molecules will be excited. The motion of molecules is extremely chaotic and any individual molecule is colliding with others at an enormous rate.

The distribution of each molecule speed is further expressed from its fundamental molecules relation as. [21]Baker, (1973)

$$N_V = 4\pi N \left( \frac{m}{2\pi k_B T} \right)^{3/2} v^2 e^{-mv^2/2k_B T}$$

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Therefore, the most probable speed of the molecule during the cause of deformations is expressed as; [20]Kittel, (1979).

$$v_{mp} = \sqrt{\frac{2K_B T}{m}}$$

9

$v_{mp}$  = most probable speed,

### 3.0 Results

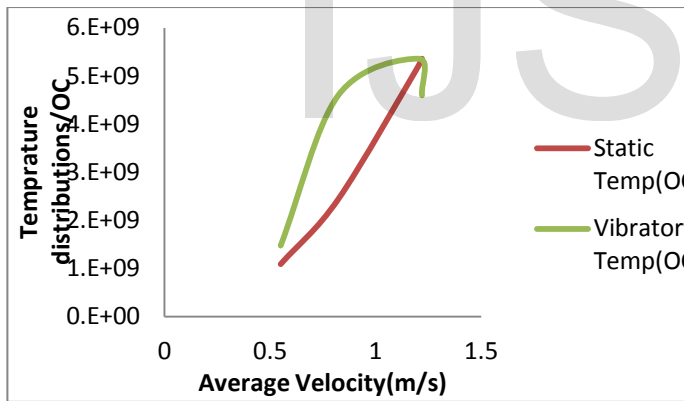


Fig. 1: Temperature distribution against average velocity of the molecules dispositions

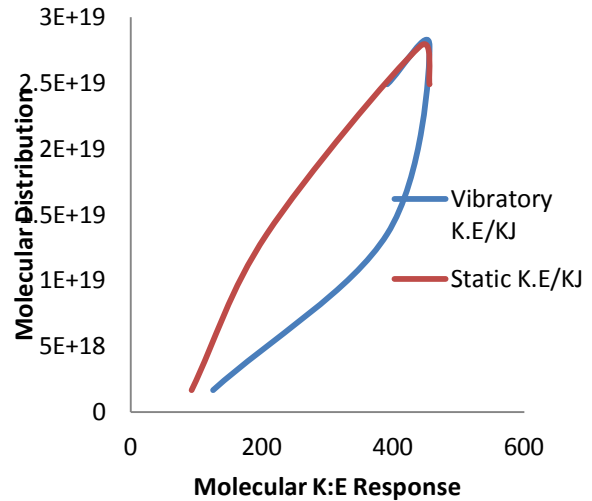


Fig. 2: The Kinetic response of the molecule as Temperature changes

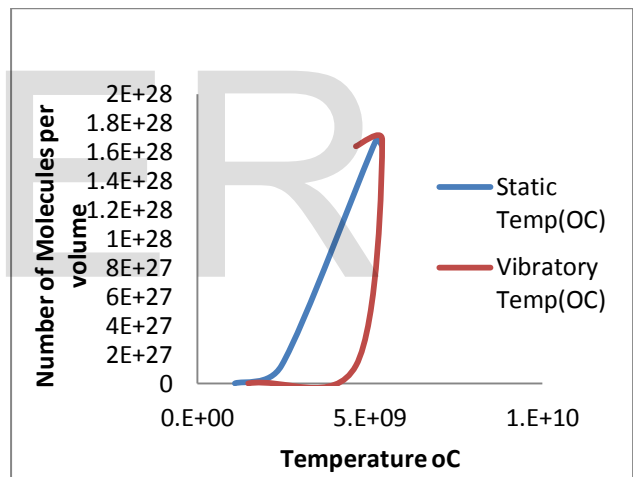


Fig. 3: Average speed response of molecules to temperature

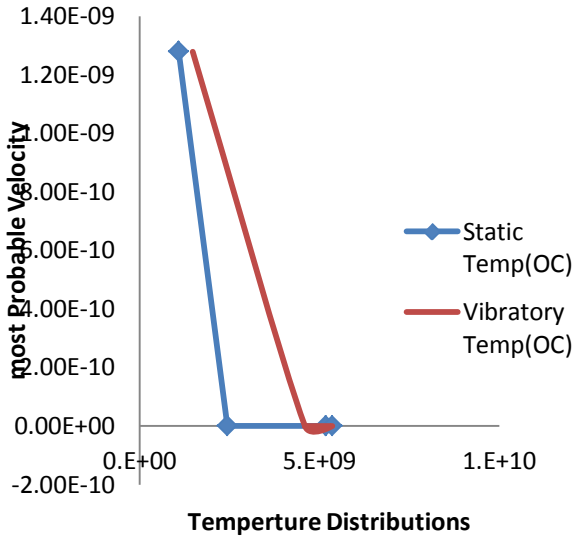


Fig. 4: Most Probable Velocity Distributions against Temperature of the system

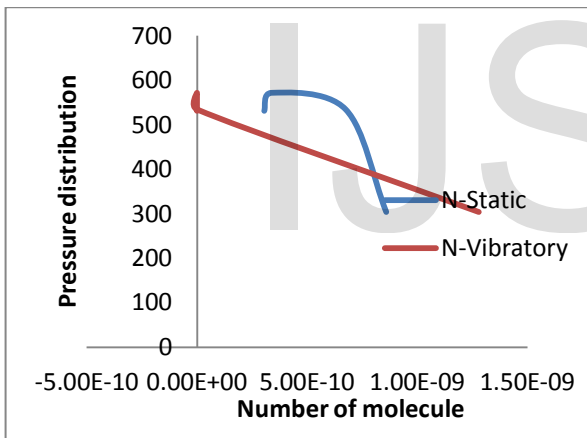


Fig. 5: Pressure Distribution effect on Molecules

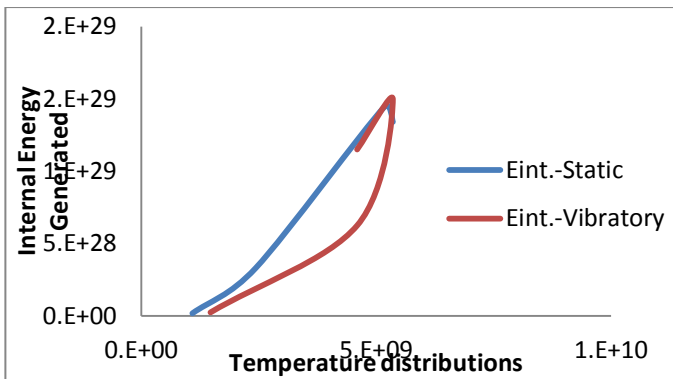


Fig. 6: Internal energy against Temperature of the materials as deforms

#### 4. Discussion

The figures 1-6 explain the various parametric deformation effects that occurred during the disposition of material molecules of experimental specimens. Figure 1 displays the temperature distribution in the material as hammer falls. It shows that the as velocity of the hammer increases as the temperature changes and this gives a linear relationship for static arrangement and a non linear relation for vibratory solidifications. The former implies that lesser energy is required for the uniform displacement of atoms per time and for the later, non-uniformities of atomic displacement per time during deformation justifies Temperature velocity non-proportionalities. Higher magnitude of energy is required for deformation of vibratory specimens as compared to that of statics. According to [22] the acceleration of vibration is responsible for the modified structure of samples given rise to higher mechanical performance, most importantly fracture strain. It could be therefore said that a vibratory sedimentary method gives a random temperature variation which makes it difficult for the molecule to easily move around to occupy the available vacant position unlike in static process while molecule are free to move about and occupy the vacant positions hence a linear temperature variations. Figure 2 presents the kinetic response of the material molecules for both processes though the static and vibratory sediment meet at a unified position where they both decrease in their kinetic energy but the kinetic energy generated affected them differently as it is reviewed that for a vibratory process molecules show more response to kinetic energy than for static process. At 400KJ a gradual decrease in molecular distribution for the vibratory process. Moreover, this is further explained in figure 3 which explains the average speed response to temperature effects of the system. As the speed changes it affect the static material directly making rise from 0°C and progresses until its peak is reached ( $1.6 \times 10^{28}$ ). On the other hand, delayed response to temperature was noticed for the vibratory process. Furthermore, most probable speed effect is presented in figure 4. This figure gives the behaviour of the static and vibratory processes as it could be seen, constant temperature is reached by static process earlier than vibratory process. This further explains the compactness solidified material on vibratory processes posses as the fine grains are more closely packed than static solidified material. Figure 5, it is observed that the pressure of the system is directly proportional to molecular displacement and consequently, the number of

molecules. A vibratory solidification process has better response to pressure than static whose response dies out before the time line. An internal energy effect of both static and vibratory solidification process is explained in figure 6. Here, changes in temperature affect the changes in the internal energy of the system. As for static process, the internal energy variations linearly increase until its peak is reached and decreases accordingly. In a vibratory process the changes in temperature causes changes in the internal energy of the process and this has noticeable effect because at negligible temperature variation, a massive effect is seen in the energy of the system until the peak is reached and both temperature and internal energy tend to decreased. This therefore explains that vibratory solidified material has a formidable strength, molecular compactness and reliability influence for deformation than static solidified specimen of the same materials.

## 5. Conclusion

Considering the nature of the above graphs and the influence of the evaluated parameters, molecular deformation is affected by kinetic energy of impacted force. Further to this, the vibrated process impounded a high average velocity of impact, vibration pressure, vibration temperature and kinetic energy of 1.22m/s, 571.48KN/m<sup>2</sup>, 5.36E+09K and 455.629KJ respectively while static process exhibit respective value of 1.2m/s, 566.71348KN/m<sup>2</sup>, 5.18E+09K and 440.8128KJ. The molecular distribution in the material morphology also relates the fact that the closeness in the molecule of the vibration process increases the number of molecular distributions up to 2.87E+19 as compared to the static process, with 2.69E+19 molecular distributions. Finally, correlating the kinetic energy of the system with the molecular distribution, it is seen that the higher kinetic energy account for the molecular distribution in a material. A vibratory process has more mechanical attractiveness than static process because it gives rise to a more closely packed system, high resistive impact strength with low response to delocalization and deformation process of materials.

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