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A Comparison of Aging Models on Alloy 6061

R.T. Shuey, J.P. Suni, M. Tiryakioğlu[1]

Alcoa Technical Center, 100 Technical Drive, Alcoa Center, PA 15069
[1]Department of Engineering, Robert Morris University, Moon Township, PA 15108

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Abstract

Recent state-variable models for aging are evaluated using Nock's data for alloy 6061. The model of Shercliff and Ashby misfits slope of strength with aging time, both underaged and overaged. Neither misfit is improved by subsequently proposed changes to strength law or to evolution law for particle radius. A nucleation-growth-coarsening model largely removes misfit underaged, but concurrently peak strength is modelled as transition from nucleation to coarsening, rather than transition from shearing to bypassing. The misfit overaged is attributed to lack of model for successor beta-prime particle. None of the models include the predecessor clusters, which show in Nock's data.

1. Introduction

During development of alloy 6061 (then called alloy 61S), J. A. Nock did an exceptionally thorough laboratory study of how the tensile properties of 1.63 mm commercial sheet responded to heat treatment and aging. He published the results [1], and they also were included in a review by W. A. Anderson [2].

Recently a number of state-variable models have been published for the dependence of yield strength on aging practice [3-7]. These models each have two components:

- Evolution of hardening precipitates during heat-treatment
- Relation between yield strength and the state of the hardening precipitates

Several of these publications used Nock's data for test or demonstration. We made our own tests of published ideas, using Nock's data. Our purpose is to decide what we can build on, and how close the state of the art is getting to useful predictive capability.

2. Fit to Shercliff-Ashby Model

Figure 1 shows Nock's data and our fit using the aging model of Shercliff and Ashby [3]. As those authors reported, the peak strengths and associated times are fit reasonably well, but there are two misfits with slope of the aging curves:

- the predicted rise to peak strength is gentler than observed
- the predicted fall-off after peak strength is steeper than observed.

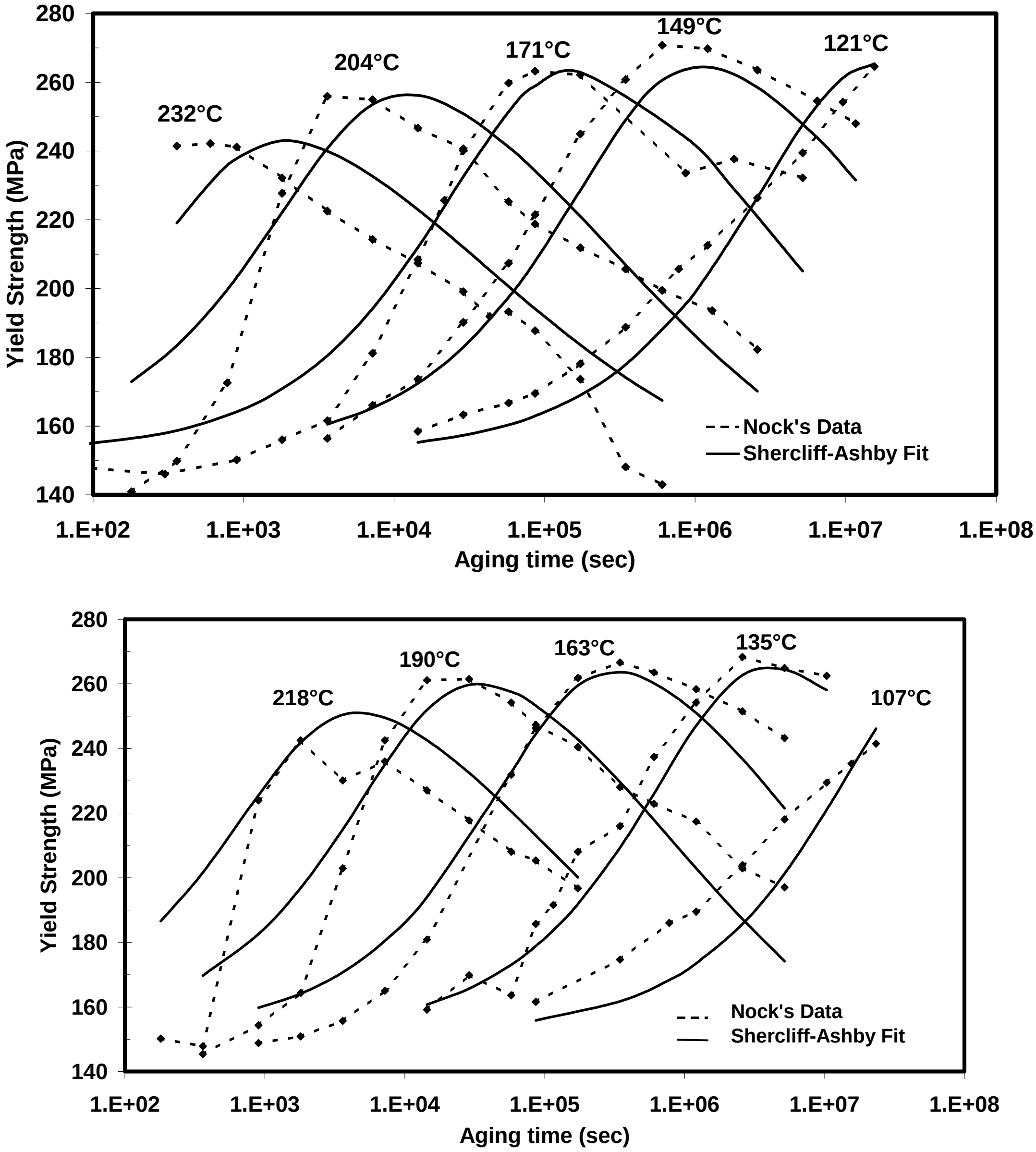

Figure 1: Fit of Shercliff and Ashby Model to Data of Nock on 6061 Aging.

Rather than the manual procedure described by Shercliff and Ashby, we used nonlinear least-squares, iteratively adjusting three parameters:

- kinetic coefficient for increase in average radius r of the β” hardening particles
- time-constant for increase in volume fraction of β” hardening particles
- critical radius for transition from particle shearing to Orowan’s particle bypassing

We held fixed a number of parameters for which adequate values could be determined *a priori* [5]: intrinsic strength, solid-solution strengthening, coefficient for strengthening by Orowan bypassing, activation energy of solute diffusion, and metastable equilibrium volume fraction β” as a function of temperature. These same procedures were followed as we went on to test other published modelling ideas, so in all cases we iteratively adjusted three coefficients to fit Nock’s data.

3. Variations on Shercliff-Ashby Model

The strength model of Shercliff and Ashby included a rather ad-hoc smooth interpolation between functional forms for particle shearing and particle bypassing. Deschamps and Brechet [4] proposed an alternative interpolation based on Friedel statistics of dislocation-particle interaction [4], and the nearly log-normal distributions reported in measurements of particle size distributions. Figure 2 compares the Shercliff-Ashby strength model to the Deschamps-Brechet model. Width of the particle size distribution is measured by Δln(r), the standard deviation of natural logarithm of particle radius. The wider the distribution, the lower and flatter the peak of strength versus average radius r, at fixed volume fraction f. The Deschamps-Brechet function approaches the Shercliff-Ashby function only for values of Δln(r) much larger than those found experimentally, or predicted by coarsening theory. For our numerical tests described below, we fixed Δln(r)=0.4.

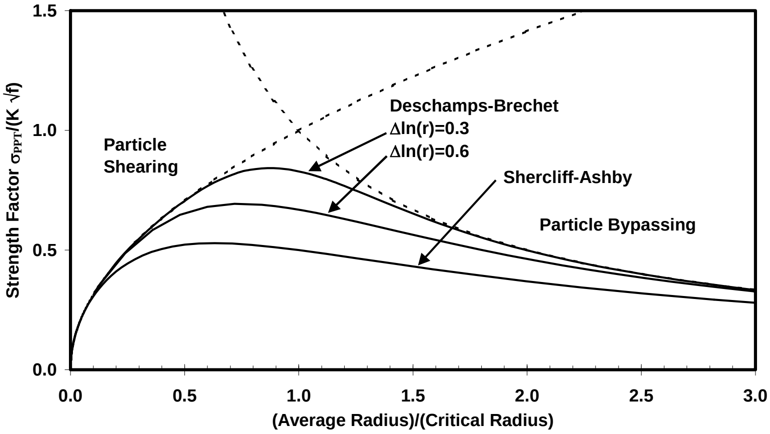

Figure 2: Strength versus Particle Radius, Shercliff-Ashby and Deschamps-Brechet Models.

For the increase of average particle radius with time, Shercliff and Ashby used the cube-root law, r~t^1/3, which is based on coarsening theory. Several later authors [6,7] proposed to use instead the square-root law, r~t^1/2, because it better fit their own TEM data on particle dimensions versus aging time.

The upper part of Table 1 identifies tests we made of these two modifications to the strength law and the radius law. Case #1 is the original Shercliff-Ashby model. Making either change individually worsened the fit (*i.e.*, increased RMS residual), while making both changes gave a slight improvement (Case #4). In all these cases we retained the exponential variation of volume fraction with time, as used by Shercliff and Ashby.

Table 1. RMS Residual from Nock's Data, for Alternative Models

	Model for Volume Fraction	Model for Radius	Model for Strength	RMS R (MPa)
1	Exponential	t^1/3	Shercliff-Ashby	13.9
2	Exponential	t^1/2	Shercliff-Ashby	15.9
3	Exponential	t^1/3	Deschamps-Brechet	15.2
4	Exponential	t^1/2	Deschamps-Brechet	13.5
5	N-G-C*, δ=0.26 J/m^2	N-G-C*	bypass/interface	14.1
6	N-G-C*, δ=0.10 J/m^2	N-G-C*	bypass/interface	12.0
7	N-G-C*, δ=0.10 J/m^2	N-G-C*	bypass - rods	11.7

*N-G-C: Nucleation-Growth-Coarsening

4. Nucleation–Growth–Coarsening (N-G-C) Models

Deschamps and Brechet also proposed to replace the separate evolutionary laws for volume fraction f and average radius r, by coupled evolutionary equations which reduce in the appropriate limits to classical nucleation, or growth, or coarsening. This was taken up by Myhr *et al*. [5], who used the Nock data as a test case.

To introduce a nucleation-growth-coarsening (N-G-C) model into our tests, we used the same procedures we have applied for a decade in contexts other than aging [5]. Deschamps and Brechet differ from us in ad-hoc guiding of the simulation from a nucleation-growth regime to a growth-coarsening regime. Myhr *et al*. differ from us in evolving an entire size distribution, as described by Kampmann and Wagner [6]. That is a more rigorous treatment of coarsening, but at a computational cost. In the present context, we believe these three N-G-C procedures perform similarly.

When we did nonlinear adjustment of three parameters to fit the Nock data, we found the critical radius in the strength model driven to zero. In this limit, both the Shercliff-Ashby and Deschamps-Brechet strength models take the functional form $\sqrt{f}/r$. The peak of strength is simulated not as a transition from shearing to bypassing, but as a transition from nucleation to coarsening. A similar interpretation of the Nock data was made by Liu *et al*. [7], but rather than a full N-G-C model they proposed simple functional forms, which we found to fit much worse than any of the models in Table 1. We do not conclude that the particles are bypassed in both underaged and overaged states. They might be sheared in both underaged and overaged states, because the “interface” shearing mechanism [7] has the same $\sqrt{f}/r$ relation to particle state as does Orowan bypassing.

By adjusting the coefficient of $\sqrt{f}/r$ while locking critical radius at zero in the strength model, we kept the number of adjustable parameters at three. N-G-C models also involve a parameter γ for the interface energy between particle and matrix. Initially we tried the value γ=0.26J/m^2 used for 6061 by Myhr *et al*. [5], but this gave a fit slightly worse than the original Shercliff-Ashby model. Upon looking at the predicted aging curves, we noticed we were doing better underaged, and worse overaged. We attributed the latter to unrealistically high γ, and indeed fit improved significantly when we tried γ=0.10J/m^2. Cases #5 and #6 in Table 1 give the statistics. Figure 3 shows how the slope underaged is significantly improved. Figure 4 shows how peak strength is now a transition from nucleation to coarsening, much as described by Deschamps and Brechet [4]. We did not continue to optimise the model value of interface energy γ.

The β” strengthening precipitates in 6061 are actually rods not spheres. Nie and Muddle generalized to rods and plates the models for both Orowan bypassing [8] and interface shearing [9]. Changing the strength model in the indicated direction gave further improvement of fit (Case # 7 in Table 1). Perhaps more realistic models do fit better.

5. Predecessor and Successor Particles

Figure 5 shows effects in Nock’s data due to predecessor clusters and successor β’ particles. The initial softening is due to dissolution of clusters formed during natural aging [10, 11]. This is not simulated by any of the models discussed. For a model to engage such practical issues as quench aging and two-step aging [12, 13], it will be necessary to model the evolution of vacancies, clusters, and their relation to nucleation of β”.

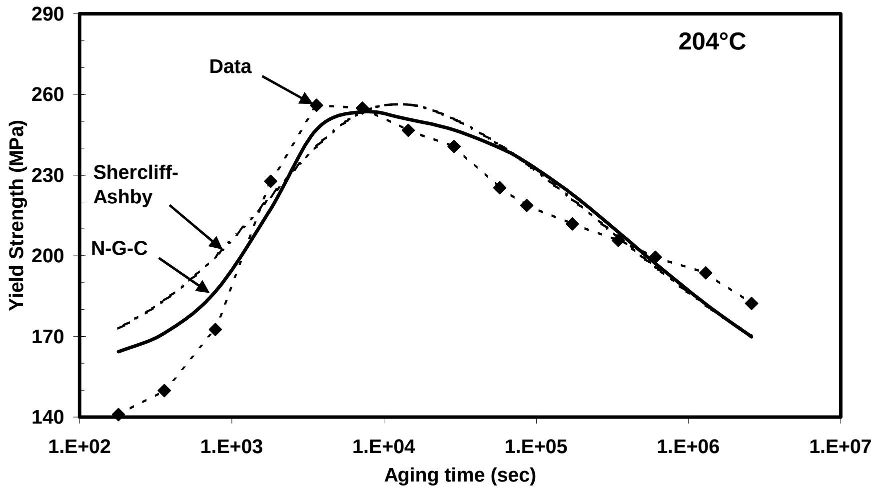

Figure 3: Fit to Aging Curve, Shercliff-Ashby and N-G-C (γ=0.10 J/m^2).

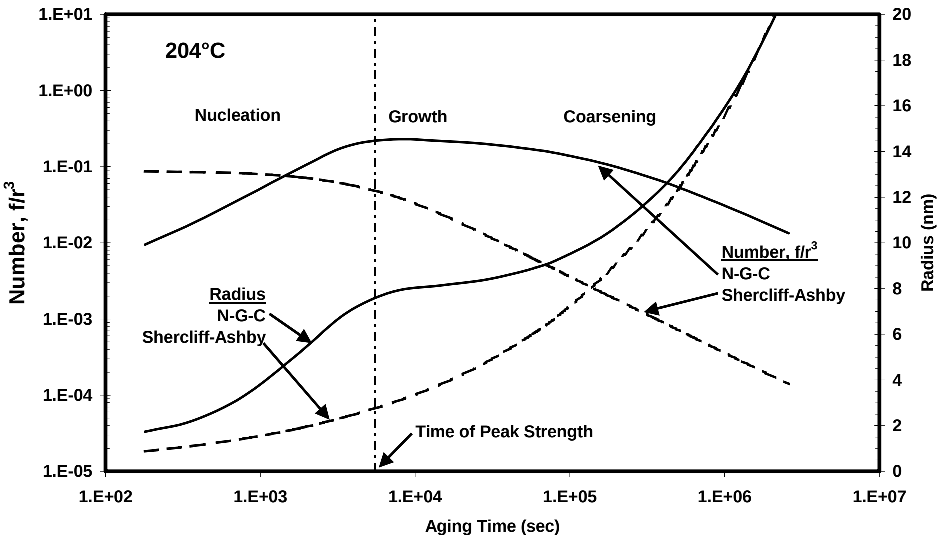

Figure 4: Particle Number and Average Radius, Shercliff-Ashby and N-G-C (γ=0.10 J/m^2).

The steep decline of strength with time at 260°C we attribute to coarsening of successor **β'** particles to nonstrengthening size. This temperature was simply omitted from Nock's data for all the fits, following Shercliff and Ashby [3]. We concur with Myhr *et al.* [5] that the presence of **β'** strengthening is the reason why all predictions fall off too steeply with overaging. Strengthening by **β'** when small is indicated by the high initial strength at 260°C (not shown), which is too close to the solvus for nucleation of **β"**. TEM data [5, 17] show **β'** to be prominent one order of magnitude of time past peak aging.

6. Conclusions

For modelling of aging to be usefully predictive, we will need to use a full N-G-C model of particle evolution, deal with coupling to predecessor and successor particles, and incorporate actual interface energy, particle shape, and shearing possibilities.

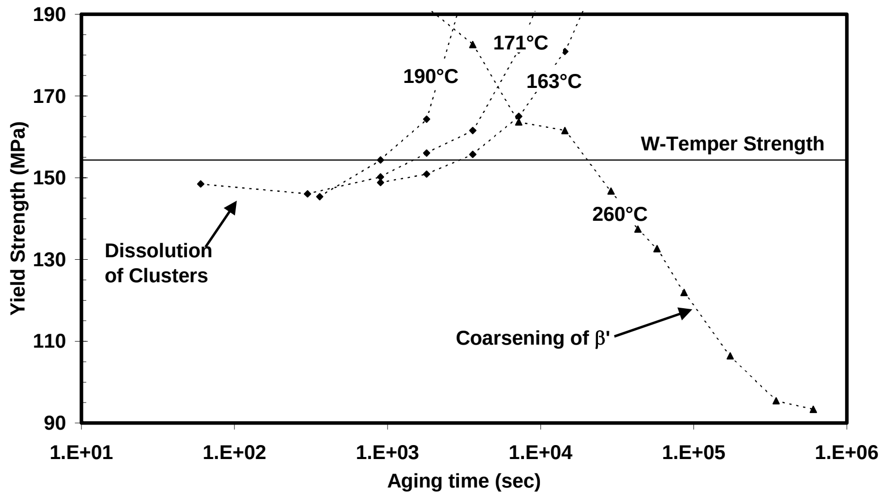

Figure 5: Effects of Predecessor and Successor Particles in Nock's Data.

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