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{311} defects in ion-implanted silicon: the cause of transient diffusion, and a mechanism for dislocation formation

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Abstract

Ion implantation is used at several critical stages of Si integrated circuit manufacturing. We show how {311} defects arising after implantation are responsible for both enhanced dopant diffusion during annealing, and stable dislocations post-anneal. We observe {311} defects in the earliest stages of an anneal. They subsequently undergo rapid Ostwald ripening and evaporation. At low implant doses evaporation dominates, and we can quantitatively relate the interstitials emitted from these defects to the tranient enhancement in diffusivity of dopants such as B and P. At higher doses Ostwald ripening is significant, and we observe the defects to undergo a series of unfaulting reactions to form both Frank loops and perfect dislocations. We demonstrate our ability to control both diffusion and dislocations by the addition of small amounts of carbon impurities.

TECHNICAL MEMORANDUM

1. INTRODUCTION

Ion implantation is the predominant technique used in production to form electrical junctions for CMOS devices in Si. A typical processing sequence shows between 12 and 18 implant steps during the "front-end" half of the process. These implants may include deep gettering, isolation (beneath the device), threshold adjustment (near the junction), guard rings, and heavy implants into poly-Si. The most critical implants are those near the source and drain, and our experiments focus on typical implant doses and energies for these steps. There is

usually a source-drain implant which is extremely high dose and low energy ($>10^{15}cm^{-2}$, $\approx$50keV), and serves the purpose of establishing a low-resistance contact to a lightly-doped region of the transistor adjacent to the gate. In most manufacturing processes, this critical junction uses a much lighter implant ($\approx10^{13}cm^{-2}$). It should be noted that although ion implantation has been very extensively studied in TEM in the past, most studies have concentrated on high implant energies, and doses much larger than that used for the critical junction.

Two issues are of primary concern: first, that defects from the implant should not extend into the active junction; and second, that the position of the implanted dopants after annealing should be well-controlled (and, preferably, predictable). This does not preclude the existence of residual (post-anneal) defects in the very heavily-doped region at the S/D, provided these defects are well removed from the depletion regions. Consequently, many manufacturers deliberately employ a strategy that leaves extended defects in this region. The precise conditions for excluding defects from the active rgion have been defined by intensive experimentation. Because of our lack of understanding, extension to new regimes (such as high-energy ion implants) is obviously problematic. A more serious issue is the control and prediction of the diffusion of implanted dopants during the anneal required to activate the implant. It has long been established that ion damage causes enhanced diffusion of dopants such as B and P. These impurities are interstitialcy diffusers, meaning (rather vaguely) that their diffusivity is enhanced in the presence of supersaturations of Si self-interstitials (e.g. during the oxidation of the Si surface). Thus transient enhanced diffusion (TED) of implanted B is attributable to elevated levels of interstitials in the implant region. Several problems exist with our knowledge of this phenomenon. Notably, the most widely accepted values for the interstitial diffusivity would allow all point defects to diffuse to the surface well before B motion was possible. Empirical solutions have been developed which use a slow Si_i diffusivity, but even these need to invoke some store for interstitials. Here, we will identify the source of interstitials driving TED, and use diffusion measurements to explain the slow-moving interstitial. In addition, we will show the mechanism by which dislocations evolve from ion damage, and establish the regimes for extended defect stability.

2. THE SOURCE OF THE INTERSTITIALS

As a model implant for a device, we used a 5 x 10^{13} cm^{-2} 40keV Si implant. This removes possible complications from the effects of the implanted species. (Comparison between Si, B and P implants suggests that this plays some role for very high doses ($\approx 10^{19} cm^{-3}$)). Figure 1 shows the microstructure seen after extremely short anneals (rapid thermal anneal RTA at 800°C, 5s). There is a high density of extended defects which resemble the "rod-like defects" well-known to occur in electron-irradiated Si, as well as a variety of other conditions (Davidson and Booker, 1970; Salisbury and Loretto, 1979; Bourret, 1987). Cross-sections show that these defects are concentrated at 500-800Å below the surface, coinciding with the projected range of a 40keV Si implant. High resolution confirms the {311} habit plane expected for these defects (Figure 2).

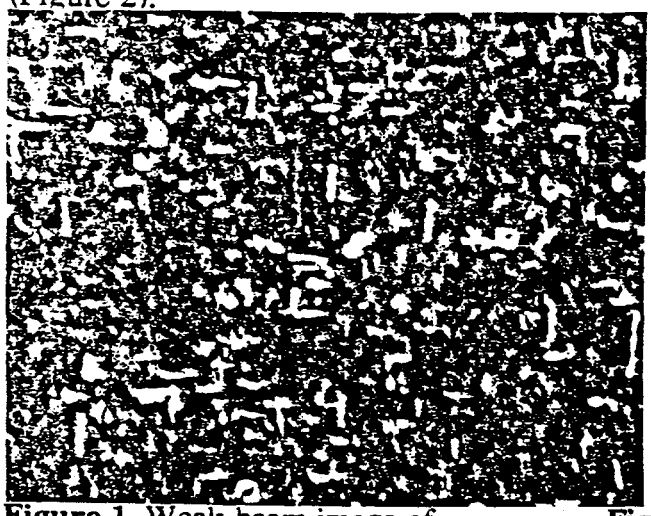

Figure 1 Weak-beam image of rod-like defects in implanted Si

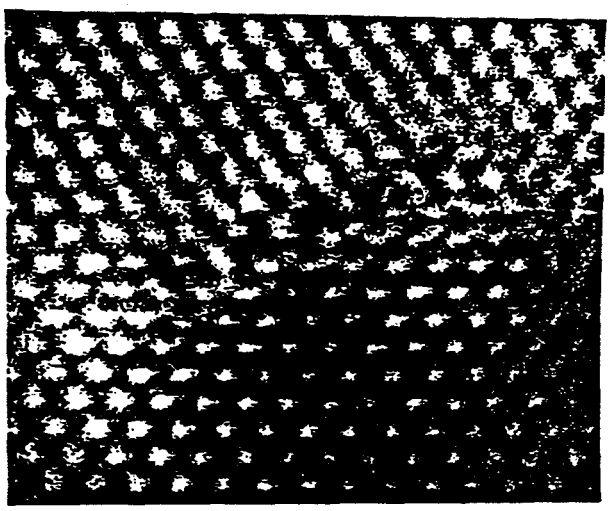

Figure 2 HREM showing {311} habit

{311} defects in Si have previously been widely reported under conditions of B or metal implantation, and oxide precipitation as well as electron irradiation. Through their extensive history they have been variously identified as B precipitates, or coesite (platelets of hexagonal SiO_2), but a consensus has emerged in the electron microscopy community that they are agglomerates of Si self-interstitials, with a local structure resembling hexagonal Si (Bourret, 1987). A structure which incorporates Si_i with 4-fold coordination of Si everywhere was proposed some time ago (Tan, Föll et al., 1980; Tan, 1981), which can be regarded as locally hexagonal. The structure determined from HREM studies of He-implanted Si (Takeda, 1991; Takeda and Kohyama, 1993)) differs from this in incorporating several additional structural units.

3. INTERSTITIAL EMISSION FROM {311} DEFECTS

Given that {311} defects consist of self-interstitial agglomerates, we can monitor the number of interstitials stored using defect counting. We measure defect widths from HREM cross-sections, and lengths and densities from plan-view weak-beam images. [Defect statistics

are obtained from particle-counting of scanned micrographs in the NIH "Image" software. Manual measurements confirm the accuracy of this routine]. Figure 3 shows the evaporation of {311} defects at different temperatures: all curves use the same $5x10^{13}cm^{-2}$ Si implant to form the initial damage. The evaporation rate is strongly temperature-dependent, with an activation energy of 3.6±0.1eV. The characteristic evaporation time for these defects has been compared directly with measurements of transient enhanced diffusion (Stolk, Gossmann et al., 1994; Stolk, Gossmann et al., 1995). The close agreement between the time to evaporate defects and the duration of the transient confirms that {311} defects are the source of interstitials causing TED. Moreover, we can now directly measure the number of interstitials injected to cause this enhancement.

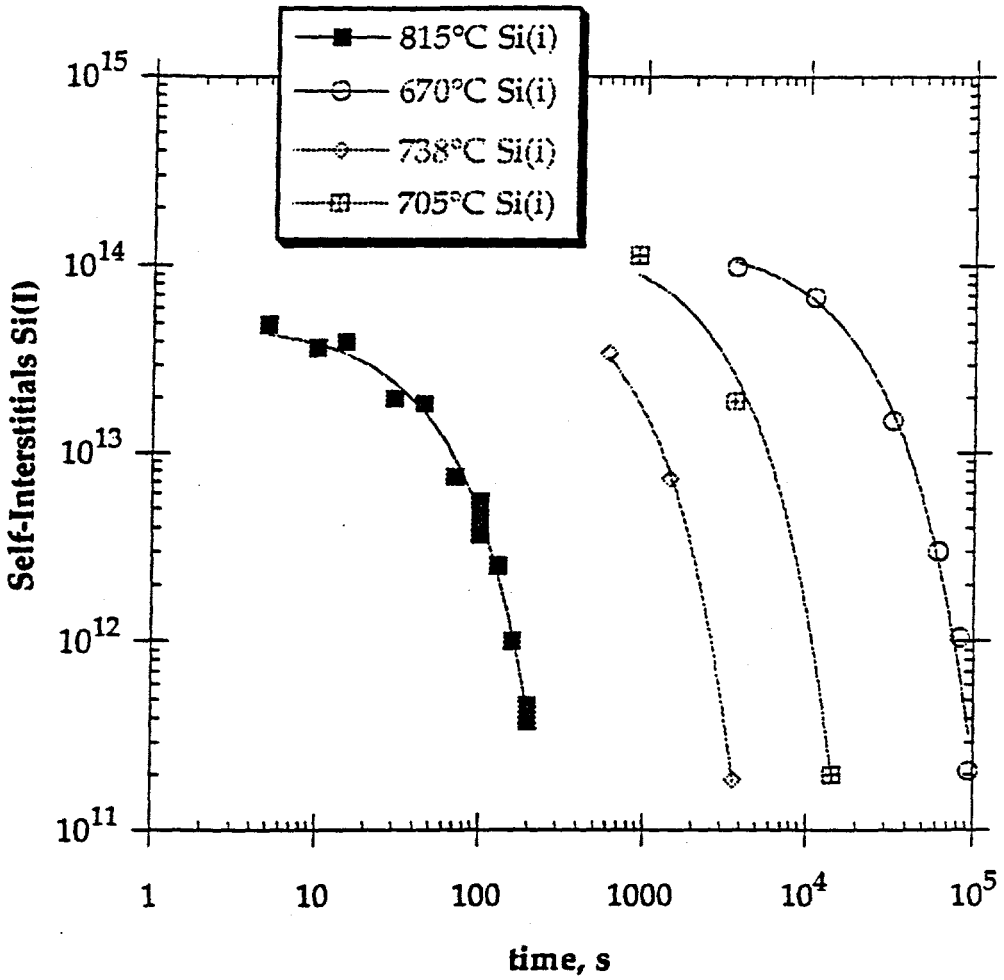

Figure 3 Evaporation of interstitials from {311} defects as a function of T

The total number of interstitials observed correlates closely with the "plus one" model. This hand-waving approximation for the post-implant point defects suggests that each implanted ion forms a cascade of ≈1000 Frenkel-pair formation events, and comes to rest in an interstitial position. Hence each implanted ion injects about 1000 vacancies and 1000 interstitials, plus one. On annealing, all Frenkel pairs annihilate, leaving the "plus one" interstitial. This picture has never been taken very seriously, despite agreement with empirical models for diffusion (Pinto, Boulin et al., 1992), and some support from experiments using pre-existing dislocations as point defect "detectors" (Listebarger, Jones et al., 1993). In Figure 4 we provide the first precise test

of the plus-one model, with the measured interstitial content of an implanted sample plotted as a function of implant dose. The close agreement suggests that Frenkel pair annihilation is extremely effective at removing the vast majority of ion damage. Deviations from "plus one" arise from subtleties in the behaviour of point defects: plus 1.4, for instance, could be attributed to a small number (0.4 per =1000) of vacancies reaching the surface.

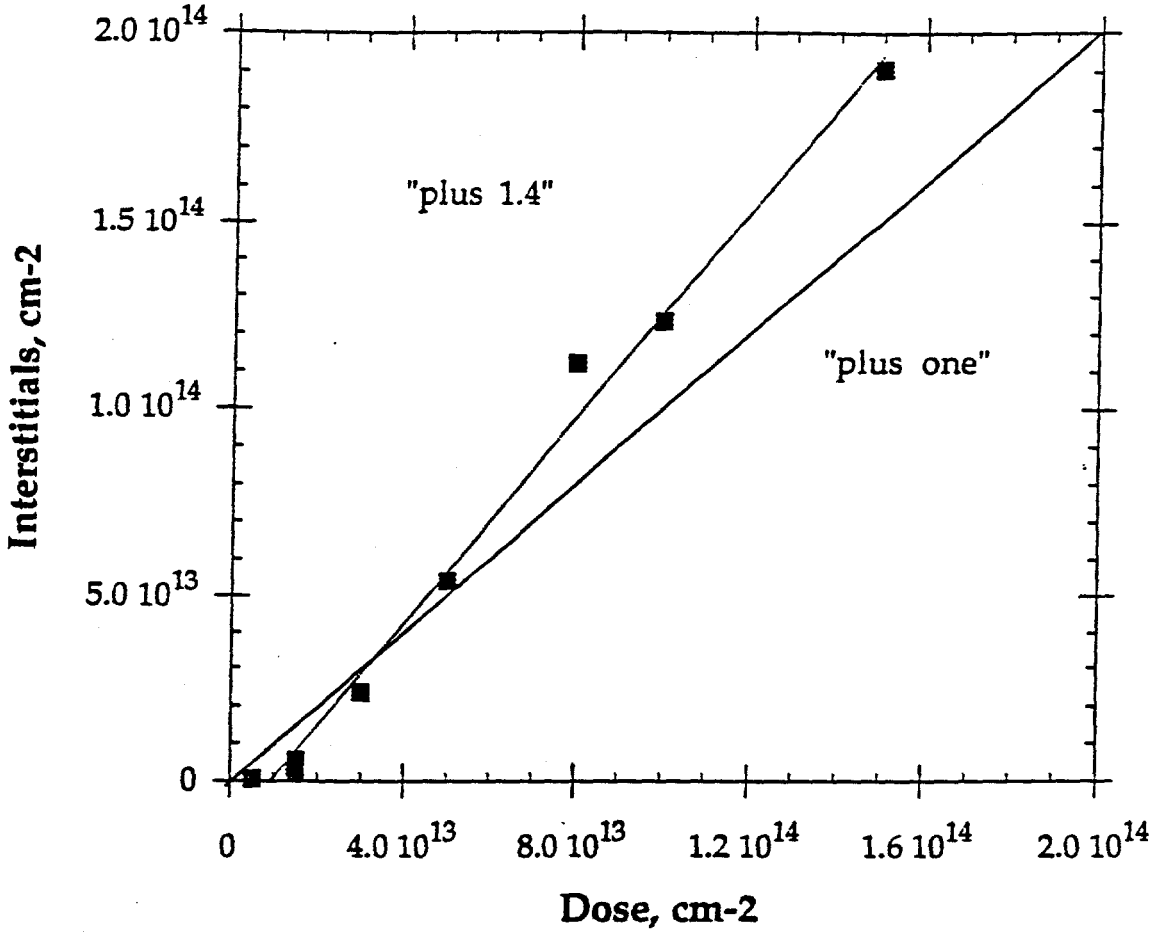

Figure 4 Testing the "plus one" model for interstitial introduction. Dose-dependence of the number of interstitials in {311} defects.

The large number of interstitials emitted from defects impacts our understanding of a key problem in Si diffusion. This is the diffusivity of the Si self-interstitial, whose reported values vary across more the 8 orders of magnitude at the processing temperature(Taylor, Marioton et al., 1989). The large concentration of interstitials, along with measurements of diffusion implicating traps (Stolk, Gossmann et al., 1995), suggest that all measurements of diffusion in Si are dominated by trap-limited diffusion of interstitials, and that traps are present at high concentrations. This in turn suggests C as a possible trap (Stolk, Gossmann et al., 1995). A consistent picture is finally beginning to emerge where trap-limited diffusion gives rise to the whole range of observed behaviour.

4. DISLOCATION FORMATION FROM {311} DEFECTS

The observation that most damage annihilates, leaving only excess interstitials, poses a new problem. It is well known that high-dose implants lead to dislocation formation. So, how do dislocations form from the relatively small point defect excess arising from the implant? On increasing the dose, we enter a regime where both {311} defects and dislocations are observed.

Fig 5 shows the microstructure resulting from a $1.5x10^{14}cm^{-2}$ 145keV Si implant annealed at 900°C, 15 minutes. The defects observed are predominantly 1/3[111] Frank loops frequently arranged in linear chains, suggesting that the loops may form from the ≈1μm long rod-like defects seen at lower doses and shorter anneals. Remnants of a {311} defect are observed connecting the Frank loop chain in Fig. 5. A plausible "unfaulting" reaction could convert the burgers vector at the {311} defect to a Frank loop (1/21<116> + 1/21<111>=1/21<777>). Despite the fact that this would require the habit plane of the defect to twist onto {111}, the observation does strongly suggest that Frank loops are forming from rod-like defects. (Previous unfaulting reactions of {311} defects during electron irradiation involved formation of perfect 1/2<110> dislocations (Salisbury and Loretto, 1979)). We expect Frank loops to further unfault into perfect dislocations, giving a dislocation formation sequence of {311}⇒Frank⇒perfect.

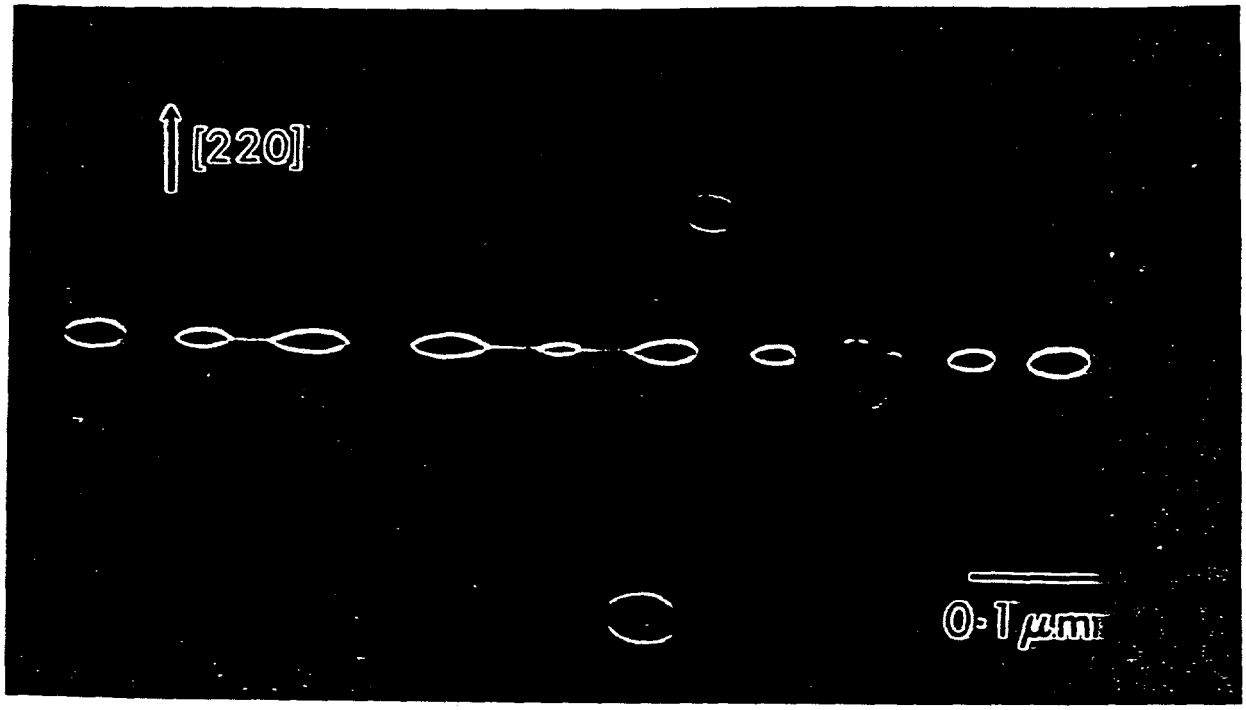

Figure 5 Frank loops forming from a {311} defect

Why do {311} defects dominate interstitial agglomeration in Si, when radiation damage in most materials (metals etc.) involves loops formation? Primarily because of the high energy of dislocations in semiconductors. The calculated energy of {311} defects is low, ≈0.5-0.9eV/interstitial (Takeda and Kohyama, 1993), consistent with tight binding of interstitials to these defects. This binding should lead to stability of these defects with respect to Frank loops for sufficiently small size. Model calculations suggest that for clusters up to 100 atoms {311} defects are more stable than the corresponding Frank loop. The system then gets trapped into a metastable situation where {311} defects grow far beyond the size where Frank loops are more stable.

In summary, we have demonstrated that interstitial evaporation from {311} defects is responsible for TED in Si. Post-implantation, Frenkel pair annihilation dominates the initial anneal, and subsequent behaviour is dictated by the small excess of interstitials, about 1.4i per implanted ion. These interstitials rapidly agglomerate into {311} defects because of the smaller activation energy for formation. Evaporation of these defects correlates perfectly with the observed diffusion transient. The diffusion is trap-limited, with the large concentration of traps implicating carbon. At high doses, the {311} defects can also give rise to stable Frank loops,

and this reaction seems to be responsible for most extended defects seen after prolonged high-temperature anneals.

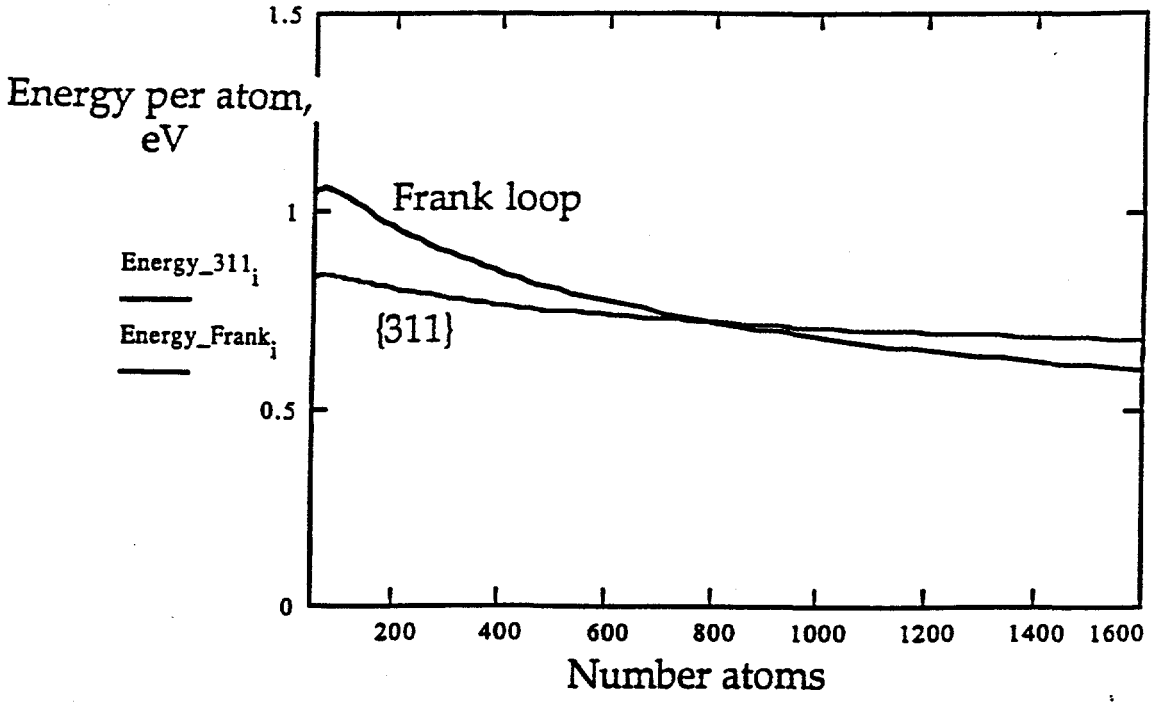

Figure 6 Calculated energies of Frank loops and {311} defects as a function of defect size. Neither the dislocation core parameter nor the {311} energy are known with any degree of certainty, but the curve does suggest why nucleation of {311} defects dominates over the more stable dislocations

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