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To: ACIS Team
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Subject: Reverse annealing and ACIS CTI increase during bakeout

Summary

This memo summarizes our expectations concerning the change in charge transfer efficiency (CTI) of ACIS detectors resulting from a bakeout. Flight experience (from September 1999; see ACIS memo 197¹) and laboratory tests (in 2002; see ACIS memo 203a) both show that if ACIS-type CCDs are irradiated at -100C by low-energy protons and then subjected to a room-temperature 'bakeout' cycle, then the bakeout itself causes additional degradation in CTI (and spectral resolution) of the devices, over and above that caused by the (pre-bakeout) irradiation itself. This phenomenon is known as reverse annealing.

Here we briefly summarize the magnitude of the reverse-annealing observed on-orbit and in the laboratory, describe a model for the phenomenon based on migration of impurities in the detector, and derive some predictions for the rate of reverse annealing as a function of bakeout duration, bakeout temperature and detector carbon concentration. We show that, given the model we adopt, chip-to-chip variations in carbon concentration can produce the observed differences between the flight- and ground reverse annealing events. We also attempt to bound the magnitude of the CTI change expected from a future bakeout of the flight instrument, allowing for plausible variations in detector carbon concentration. Finally, we consider the evidence for and against the adopted model and identify possible additional tests of it.

1 Observed Bakeout-Induced CTI Changes

Reverse annealing was observed in the flight CCDs in 1999 and in laboratory tests in 2002. Key experimental parameters and results are listed in Table 1. In both flight and laboratory events, the CCDs were at -100C during both irradiation and CTI characterization, and the bakeout was nominally of 8 hours duration with a maximum focal plane temperature of +30C.

As described below, our model for the reverse annealing process predicts that the increase in CTI resulting from bakeout is proportional to the (pre-bakeout) increase in CTI produced by the irradiation. It is useful to define the proportionality constant, R , as follows:

$$R \equiv \frac{CTI_{post-bakeout} - CTI_{post-irradiation \& pre-bakeout}}{CTI_{post-irradiation \& pre-bakeout} - CTI_{pre-irradiation}} \equiv \frac{\delta CTI_{bake}}{\delta CTI_{rad}} \quad (1)$$

¹ACIS memos are available at <http://space.mit.edu/ACIS/iacis.html>

Event	Detector	Bake Time/Temp.	Pre-irr. CTI ^a	Post-irr. CTI ^a	Post-bake CTI ^a	Bakeout-induced CTI ratio R^b
On-orbit (1999)	S2(w182c4; FI)	8h/+30C	< 0.3	20.5	27.5	0.32 ± 0.01
On-orbit (1999)	S3(w134c4; FI)	8h/+30C	0.39 ^c	0.55	0.60	0.31 ± 0.36^c
Lab Test (2002)	w183c3; FI	8h/+30C	< 0.3	11.2	27.8	1.48 ± 0.03

Table 1: Summary of On-orbit and Ground Test Experience with Bakeout

Notes:

a: CTI in units of 10^{-5} per transfer at -100C. b: R is proportionality constant relating the pre-bakeout, radiation-induced CTI change to bakeout-induced CTI change, i.e., ratio of (column 6 - column 5) to (column 5 - column 4). c: The large uncertainty results from the uncertainty in S3's pre-irradiation CTI at -100C. See text.

It is worth noting that the value of R will depend on the details of the bakeout (duration and temperature) and also on characteristics of the CCD material. If the bakeout parameters, radiation conditions and detector characteristics are the same in both flight and ground tests, then identical values of R should be measured. ²

The last column of Table 1 shows that the value of R is indeed the same for both flight detectors, though the errors on the value for S3 are large. However, the flight and laboratory measurements of R differ by a factor of almost five. We consider the interpretation of this discrepancy below.

The effects of both radiation and the on-orbit bakeout on the back-illuminated (BI) S3 detector were small, and the large relative uncertainties in these effects may deserve comment. No on-orbit measurements of S3 CTI at -100C were made prior to radiation exposure in August 1999, and no ground measurements of S3 CTI at -100C are available. Ground data and post-irradiation on-orbit S3 CTI measurements at -110C agree within the ($\sim 10\%$) errors of those measurements. The value for pre-irradiation S3 CTI at -100C listed in Table 1 was obtained from obsid 62411, which occurred after some on-orbit radiation exposure but before the on-orbit bakeout. The associated (1-sigma) relative uncertainty in this measurement is large ($\sim \pm 33\%$), and the relative uncertainty on the radiation-induced change in CTI is even larger ($\sim 80\%$). Moreover, the bakeout changed S3 CTI at less than the 2-sigma level. As a result, the uncertainty in the fractional increase in radiation-induced CTI resulting from bakeout is quite large for S3.

2 Model for Reverse Annealing

Our model for bakeout-induced degradation of CTI ('reverse annealing') is the one proposed by Kono [2, 3] and discussed briefly in MIT ACIS memo 203a. In this model the reverse annealing results from the behavior of carbon impurities during the irradiation and subsequent bakeout.

2.1 Qualitative Description of the Model

Irradiation of the cold detector by soft protons produces two effects. First, silicon atoms are displaced, leaving lattice vacancies. Both the displaced silicon interstitials and the vacancies are highly mobile. Note that these particular vacancy-related defects degrade CTI independently of any subsequent bakeout. The CTI change occurring in this process is labelled δCTI_{rad} in this memo.

²One may also think of the bakeout as amplifying the initial, radiation-induced CTI, so that $CTI_{post-bakeout} = G \times (CTI_{post-irradiation \& pre-bakeout} - CTI_{pre-irradiation})$. Then $G = 1 + R$.

The second effect of the irradiation of the cold detector is to move carbon impurities from so-called substitutional lattice sites (where they substituted for silicon atoms) to interstitial sites. This process actually proceeds in two steps: the radiation displaces silicon atoms (as described above) and the mobile silicon atoms exchange places with substitutional carbon atoms through what is known as the Watkins replacement reaction [3]. The result is a radiation-induced population of interstitial carbon atoms. These atoms are *not* mobile at typical ACIS detector operating temperatures. Although there is an electron trap associated with interstitial carbon, this trap does not compromise CTI because its emission time is believed to be too short to do so under ordinary ACIS operating conditions.

Note that in this picture, the number of vacancy-related defects, on the one hand, and the number of interstitial carbon atoms, on the other, should each be proportional to the non-ionizing energy dose imparted to the detector during the initial proton irradiation. It follows that the number of interstitial carbon atoms produced should be proportional to the initial CTI change caused by the radiation.

Bakeout of the irradiated detector to +30C produces an additional degradation in CTI (i.e., reverse annealing) because the interstitial carbon atoms become mobile at this temperature. This change in CTI is labelled δCTI_{bake} in this memo. Once mobile, the interstitial carbon is able to react with (substitutional) impurities in the lattice to form new carbon-related defects and associated new electron traps. For ACIS the most important such impurities seem to be substitutional carbon and phosphorous. The so-called C_iC_s and C_iP defects each have electron traps which can have a serious effect on CTI. (Remarkably, the energy level of a trap associated with C_iC_s is nearly identical to that associated with the oxygen-vacancy defect produced in the initial radiation [8].)

In a bakeout of any finite duration, some fraction of the radiation-induced C_i will be converted into these defect complexes. This conversion, or reverse annealing, is assumed to be a first-order process, so the density of C_i will drop exponentially with a characteristic time constant. The density of new defects (and the bakeout-induced CTI) will rise at a complementary rate, eventually reaching a maximum value asymptotically as the reverse-annealing process eventually converts all of the C_i into other defects. Note that the level of the asymptotic, bakeout-induced CTI change, $\delta CTI_{bake,max}$, is proportional to the initial non-ionizing energy loss (and therefore to δCTI_{rad}) and also proportional to the initial density N_s of C_s .

2.2 Rate of Reverse Annealing

The rate of the reverse annealing process can be estimated in this picture as follows. At fixed temperature, interstitial carbon (C_i) anneals to C_iC_s via a first order process. That is, the density N_i of C_i varies with time t as

$$\frac{dN_i}{dt} = -k(T) \times N_i \quad (2)$$

where the rate coefficient k for this process is proportional to the product of N_s , the initial density of C_s , the interaction cross-section between C_i and C_s , and the flux of migrating C_i in the silicon during the bakeout.³ The latter factor leads to variation of $k(T)$ with temperature T as [4]

$$k(T) = k_0 \exp(-E_{act}/k_B T) \quad (3)$$

³We assume that only a small fraction of the C_s are converted to C_i by the radiation. If a significant fraction, say, f , of the C_s are converted to C_i , then k_0 includes a factor $(1 - f)$. Interestingly, in the limit of extremely high radiation dose, $f = 1$ and formally the reverse annealing is completely suppressed.

Here E_{act} is a so-called migration enthalpy characteristic of the C_i transport process and k_B is Boltzmann's constant.⁴

In this picture, at constant temperature the interstitial density N_i falls exponentially with time with a time constant $\tau(T) = 1/k$. Since each C_i is converted into a single new electron trap, the new trap density (and, hence, the additional CTI due to the bakeout) grows with time t during the bakeout as

$$\delta CTI_{bake}(t) = \delta CTI_{bake,max}(1 - \exp(-t/\tau(T))) \quad (4)$$

The time-dependence of CTI during the bakeout is thus characterized by two parameters, each of which depends in turn on a variety of other quantities. The (asymptotic) amplitude $\delta CTI_{bake,max}$, is proportional to both the initial radiation dose (and hence δCTI_{rad}) and the initial carbon concentration in the CCD, N_s . The time constant $\tau(T)$ depends on the temperature T , the migration enthalpy E_{act} and (inversely) on N_s . Note that E_{act} is characteristic of the interaction between an interstitial carbon atom and the silicon lattice and is thus (approximately) independent of the details of the detector material; in this sense the temperature dependence of the annealing is independent of these details. On the other hand, at any particular temperature, the amplitude of the reverse annealing depends on both the radiation dose and the carbon concentration in the detector, while the time constant depends on the carbon concentration (for sufficiently low doses.)

2.3 Temperature Dependence of the Annealing Rate

Reasonably precise values for E_{act} are available in the literature. From [8] we find $E_{act} = 0.73 - 0.75$ eV, a range of values recommended by [4] which we adopt. Values of k_0 for n-type silicon range from $1 - 2 \times 10^8 \text{ s}^{-1}$ for float-zone samples with C and P concentrations comparable to those believed present in the ACIS detectors.⁵ These are equivalent, given the values of E_{act} adopted above, to time constants at $T = 300\text{K}$ of 18000 to 54000 s. For a sample much richer in carbon, [5] show annealing data implying a time constant of 7200 s.

Finally, our own laboratory measurements showed no significant additional reverse annealing when an initial 8-hour bakeout at +30C was followed by an additional 16hr bakeout at +25C. From these data (CTI measurements C9, C10 and C11 in ACIS memo 203a) we estimate a 90% confidence upper limit of $\tau < 21000\text{s}$ for the laboratory test device. For reasons described below, it is plausible that the flight detectors may have time constants roughly a factor of 3 longer than the laboratory device just described, so the flight detectors may have time constants (at +30C) as large as 63000s.

Figure 1 shows normalized CTI increase (i.e., $\delta CTI_{bake}/\delta CTI_{bake,max}$) as a function of time for several bakeout temperatures and a range of time constants. The figure shows that, regardless of the assumed time constant (in this range) the total bakeout-induced CTI change is very nearly the same for a +10C, 300 ks bakeout as for a +20C, 150ks bakeout. In particular, for the long time-constant case, the expected (normalized) CTI changes are 0.45 and 0.48 for the two bakeout scenarios, respectively. For the short time constant case the normalized CTI changes are both greater than 0.99.

⁴A further complication arises if (as seems likely) other processes (e.g., $C_i + P \rightarrow CiP$) also contribute to the reverse annealing of C_i . In this case, the total annealing rate is the sum of the rates for the various component processes. That is, the values of k_0 for the relevant processes must be added.

⁵The ACIS detectors were fabricated from high-resistivity ($\sim 5k\Omega\text{-cm}$) p-type float-zone silicon with a carbon concentration of $\sim 10^{16} \text{ cm}^{-3}$. The n-type buried channel (in which charge transfer occurs) has a peak phosphorous concentration of $\sim 7 \times 10^{16} \text{ cm}^{-3}$.

2.4 Dependence of Reverse Annealing on Carbon Concentration

As noted in the previous section, in this model the concentration of carbon impurities, N_s , has a significant effect on the reverse annealing process. To determine whether chip-to-chip variations in N_s might be responsible for the different values of the R parameter noted above, we consider a situation in which two otherwise identical detectors, which have different values of N_s , are irradiated and then subjected to identical bakeouts.

How does the ratio of the R parameters of these two detectors (call it R_{ground}/R_{flight}) depend on the ratio of carbon concentrations, $N_{g:f} \equiv N_{s,ground}/N_{s,flight}$? Since $\tau \propto N_s^{-1}$ and $\delta CTI_{bake,max} \propto N_s$, it follows that

$$R_{ground}/R_{flight} = N_{g:f}(1 - x)/(1 - x^{1/N_{g:f}}) \quad (5)$$

with $x \equiv \exp(-t/\tau_{ground})$ and t is the duration of the bakeout. Note that Equation 5 holds even if the incident radiation fluences of the two detectors differ. This is so because R is normalized to be independent of the incident radiation fluence.

Figure 2 shows R_{ground}/R_{flight} plotted as a function of carbon concentration ratio $N_{g:f}$ for two extreme values of τ_{ground} (given a temperature of $T=303K$). The assumed bakeout duration, 8 hours, matches the bakeouts described in Table 1. Note also that the ratio of R parameters is varies non-linearly with $N_{g:f}$: a given fractional variation in $N_{g:f}$ produces a larger fractional variation in R .

Note in particular that for $2.6 < N_{g:f} < 3.4$, the observed value of $R_{ground}/R_{flight} = 4.6$ is reproduced by this model. Wafer-to-wafer carbon concentrations variations of a factor of 3 are not unexpected for ACIS devices.⁶ It appears that in this simple model, then, that variations in carbon concentration can explain the difference in bakeout effects observed in flight and in laboratory tests.

It must also be noted that if C_iP defects are an important component of the bakeout-induced CTI change, then R_{ground}/R_{flight} will vary less rapidly with changes in carbon concentration than is indicated by equation 5. In particular, for constant phosphorous concentration⁷, the time constant associated with C_iP formation will be same for all devices, independent of the carbon concentration. Thus the value of $\delta CTI_{max,bake}$, and R_{ground}/R_{flight} associated with C_iP formation will vary (only) linearly with the carbon concentration parameter $N_{g:f}$. The net result is that somewhat variations in carbon concentration would have to be larger than those implied by Figure 2 in order to reconcile the flight and ground results. If *all* of the bakeout induced CTI change were the result of C_iP formation, for example, then $N_{g:f} = 4.6$ would be required to reconcile flight and ground results.

3 Implications for a future ACIS bakeout

If this model is correct, then the carbon concentration in flight detector S2 is relatively small, and the annealing time constant is correspondingly long. In fact, in this case the time constant of S2 is long enough that the 1999 on-orbit bakeout will *not* have been long enough to have allowed the reverse annealing of the 1999 radiation damage to have reached its asymptotic value. As a result, this model predicts that a subsequent ACIS bakeout would induce additional reverse annealing of the 1999 radiation damage, as well as reverse annealing of radiation damage accumulated between the 1999 ACIS bakeout and the present.

Predictions for the effect of a second ACIS bakeout on two flight detectors, for each of two assumptions about the annealing time constant, are listed in Table 2. We have adopted the +20C,

⁶J. A. Gregory, MIT Lincoln Laboratory, private communication.

⁷Phosphorous concentration is determined by the buried-channel and “trough” implants during detector fabrication, and should thus be much more uniform, from device to device, than the carbon concentration.

$N_{g:f}^a$	τ^b (ks)	R_{1999}	$R(t \rightarrow \infty)^e$	$\delta CTI_{rad}^{c,d}$		$\delta CTI_{bake}^{c,f}$ '04		Current CTI^c	Predicted CTI Change $\frac{CTI_{postbake}}{CTI_{prebake}}$
				'99	'99-'04 ^g	resid '99	'99-'04		
<i>S2:</i>									
2.6	147	0.32	0.76	1	0.24	0.36	0.12	1.57	1.26
3.3	62	0.32	0.45	1	0.24	0.12	0.10	1.57	1.14
<i>S3^h:</i>									
2.6	147	0.32	0.76	1	0.24	0.36	0.12	3.97	1.12
3.3	62	0.32	0.45	1	0.24	0.12	0.10	3.97	1.06
<i>w183c3, hypothetically on-orbit:</i>									
1.0	57	1.48	1.98	1	0.24	0.46	0.44	2.72	1.33
1.0	19	1.48	1.51	1	0.24	0.03	0.36	2.72	1.14
<i>Hypothetical carbon-rich FI detector:</i>									
0.33	19	5.84	5.94	1	0.24	0.10	1.43	7.08	1.22
0.33	6.5	5.87	5.94	1	0.24	0.07	1.43	7.11	1.21
<i>Hypothetical carbon-poor FI detector:</i>									
10	567	0.026	0.20	1	0.24	0.005	0.01	1.27	1.02
10	194	0.066	0.20	1	0.24	0.072	0.026	1.31	1.08

Table 2: Predicted Change in CTI due to bakeout for various ACIS detectors

Notes:

a: Assumed ratio of carbon concentration, “ground:flight.” b: Assumed annealing time constant at +20C; scaled from limits on w183c3 τ . c: CTI in units of that immediately prior to 1999 +30C bakeout d: Pre-bakeout CTI change due to pre-1999-bakeout irradiation (δCTI_{rad}). e: Predicted value of R parameter for an infinitely long bakeout. f: Assuming 2004 bakeout is either 150 ks at +20C or 300 ks at +10C. g: Two-thirds of this component of CTI change is due to a final, unprotected passage of the detectors through the radiation belts after the 1999 +30C bakeout. h: A large fraction of S3 CTI was present at launch and is unaffected by bakeout. Radiation and bakeout-induced CTI changes for S3 are small and very uncertain; see Table 1.

150 ks bakeout scenario for these calculations, but the only number in Table 2 affected by this assumption is the time constant τ . As discussed above, the predicted effect of the bakeout would be (almost exactly) the same if the +10C, 300 ks bakeout were assumed.

To illustrate the consequences of larger variations in carbon concentration, we also list bakeout-induced CTI change predictions for three other hypothetical cases in Table 2. In making these predictions we suppose that all detectors received the same radiation dose as S2, and that all would have shown the same CTI as S2 just before the 1999 bakeout. One such case is predicts what might have happened if w183c3, a detector used in ground tests, had been flown on ACIS. Two other cases show detectors with much higher and much lower carbon concentrations, respectively. The table shows that, except for the carbon-rich detector, these hypothetical cases could easily represent actual ACIS focal plane detectors, since they have would currently show CTI ranging from 80% to 170% of that of S2, which is comparable to the range of CTI shown by the ACIS focal plane detectors. Note, however, that it is not known, at this writing, how much of this CTI variation is due to intrinsic detector differences and how much is due to variation of the initial radiation dose over the ACIS focal plane.

4 Conclusions & Possible Additional Investigations

We have summarized our on-orbit and laboratory experience with reverse annealing of ACIS detectors. We examined a simple model, originally suggested by others [2, 3], for the reverse annealing

process, and found that it plausibly accounts for the laboratory data we have on the the rate of the reverse annealing process, as well as for the (long-puzzling) differences in the magnitude of reverse annealing observed in the flight- and laboaratory-test detectors. The model attributes these variations to detector-to-detector variations in the concentration of carbon in the silicon from which the ACIS detectors were fabricated. The model predicts that any ACIS bakeout now being considered is likely to increase the CTI of front-illuminated detectors by as little as a few percent to as much as about one-third. The back-illuminated detector CTI may increase by of order 5-10%, but the predicted change is more uncertain than that for the FI detectors (the BI predicted change is significant at about the $2 - \sigma$ level), and is in any event very likely of less consequence because the absolute level of the BI detectors' CTI is roughly an order of magnitude smaller.

Although the model seems to account for all of our observations about reverse annealing in ACIS detectors, the evidence for it is almost all circumstantial. In addition to the qualitative statements made in the preceding paragraph, we may also note the following:

- Wafer-to-wafer carbon concentration variations of a factor of 3, which are required to explain the observations, are thought to be plausible.
- The model predicts variations in the (post-bakeout) CTI in roughly the range observed in the ACIS flight detectors, though the observed variation might also be due to spatial variations in focal-plane radiation fluence. Room-temperature radiation tests on four ACIS detectors may also show variation in radiation sensitivity of about the implied magnitude. It must be acknowledged that some of that variation may be due to systematic experimental errors. See ACIS memo 205.
- Some of the defects produced by the revese annealing in this model should be bistable [7, 8]. We see some evidence for this in detailed analysis of ground test data [1].

We also summarize some caveats concerning this intepretation:

- The model predicts that carbon concentration is positively correlated with (post-bakeout) radiation sensitivity, and requires that at least S2, and possibly most of the other flight detectors, have lower carbon concentration than the ground test device w183c3. On the other hand, there is some evidence (see ACIS memo 205) that w183c3 is the least radiation-sensitive of the five detectors subjected to (warm or cold) ground irradiation tests. Thus it appears that most of the flight detectors must have lower carbon concentration than all of the ground detectors used in radiation tests to date. This state of affairs need not be a coincidence (the flight detectors were carefully selected for CTI and cosmetic quality, though not for radiation tolerance) but should be borne in mind when considering the plausibility of this model.
- Rather larger carbon concentration variations than those predicted in Figure 2 (as large as a factor of 4.6) are required if C_iP defects are an important contributor the bakeout-induced CTI increase.

Finally, several steps might be taken to test the model. For example, one might:

- Assay the carbon content of ACIS wafers to check the actual wafer-to-wafer variability.
- Characterize the chip-to-chip variation in radiation sensitivity and/or reverse annealing behavior of a larger sample of ACIS sibling devices more systematically than we have yet done.

- Conduct laboratory tests to determine i) the temperature dependence of the reverse annealing to see if it matches that expected for carbon migration and/or ii) whether the damage sites can be annealed away at elevated (+200C) temperature. The latter test might be done without additional radiation exposures, using devices that have already been irradiated.
- Attempt to compute the relative densities of primary traps (that is, those associated with OV and VV centers) and carbon interstitials produced by the incident radiation. Existing simulations (e.g., SRIM) might be capable of addressing this question.

It is not clear how many of these tests are actually practical.

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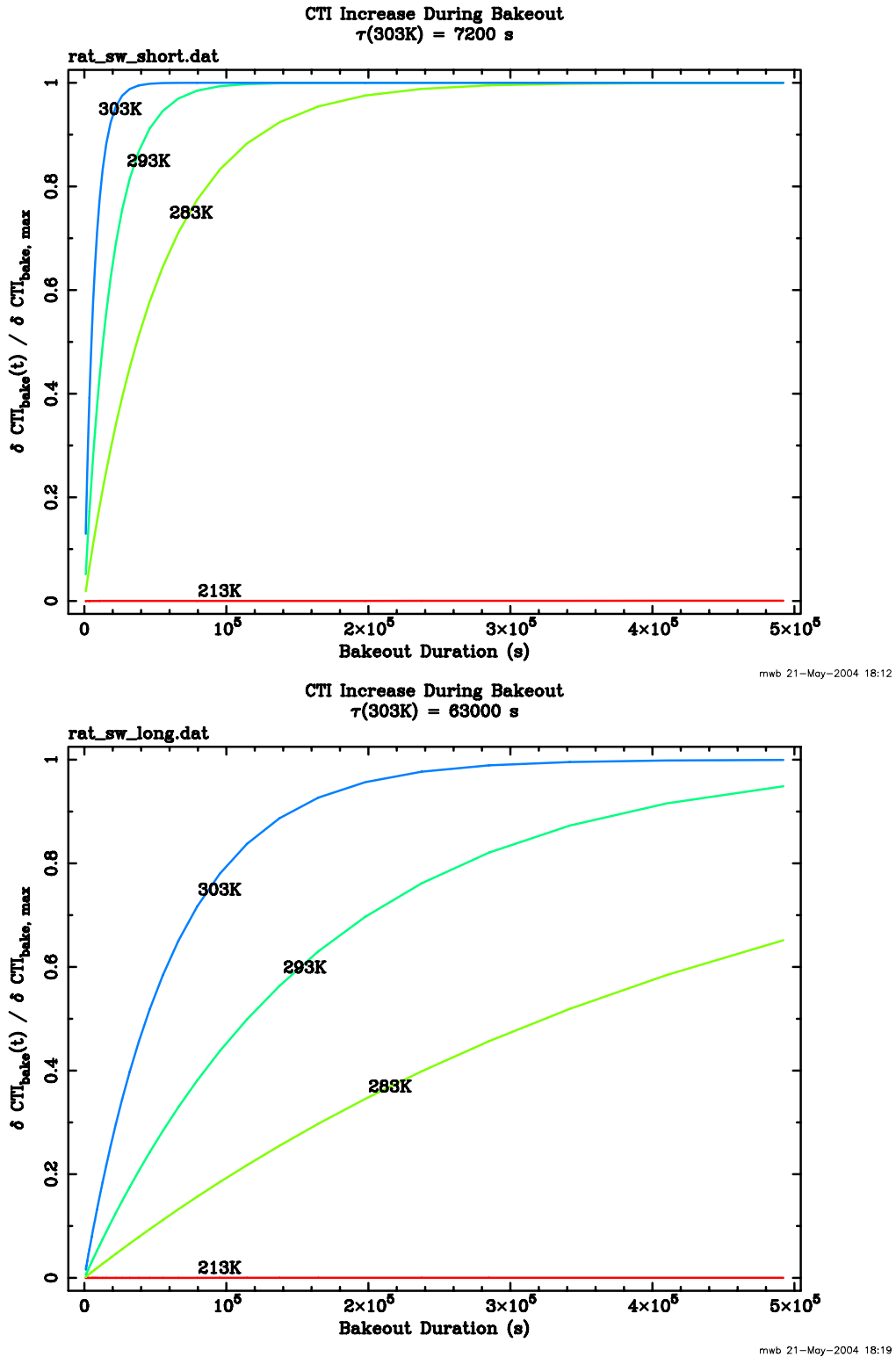
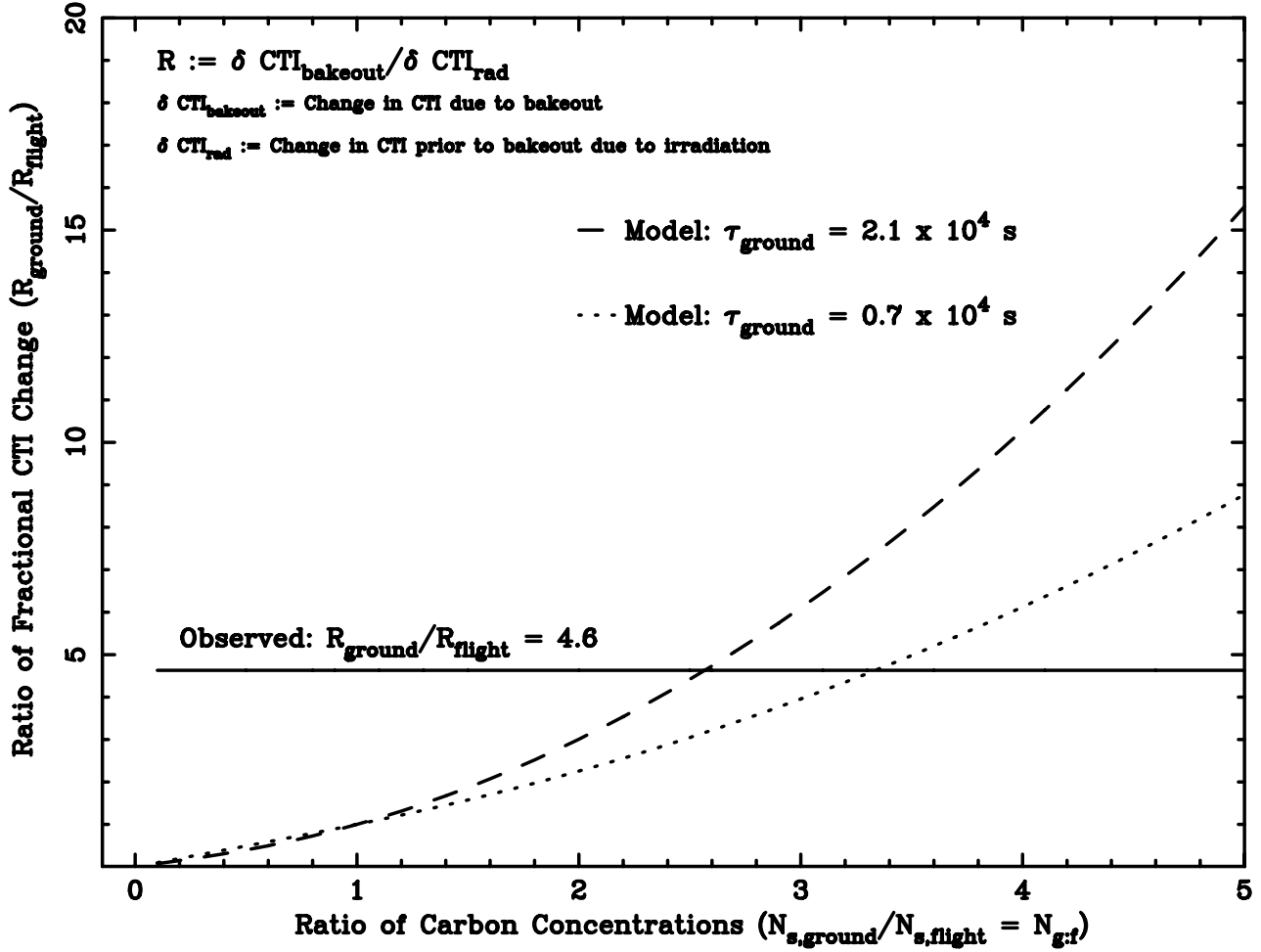


Figure 1: Model predictions for (normalized) increase of CTI with time during bakeout. The two panels show results for assumed reverse annealing time constants at 303K of 7200s (top panel) and 63,000s (bottom panel). These are extremes which probably bracket plausible values. For either value of the time constant, the bakeout-induced CTI increase is roughly the same for a ($T=293K$, $t=150 \text{ ks}$) bakeout as for a ($T=283K$, $t=300 \text{ ks}$) bakeout. The predicted value of $\delta CTI_{bake} / \delta CTI_{bake,max}$ at the end of the bakeout varies by factor of two as the assumed time constant varies between these extremes.

**Effect of Carbon Concentration on Bakeout-Induced CTI Change
8-hr, +30C Bakeout**



CO= 4.630

Figure 2: Model predictions for the ratio of R parameters for a ground and a flight detector with different carbon concentrations, as a function of the ratio of carbon concentrations of the two detectors. The observed value of $R = 4.6$ is reproduced by the models if the carbon concentration ratio is in the range 2.6 – 3.3, depending on the assumed value of the annealing time constant for the ground detector.