Heat load variations on web substrates as seen by deposition modelling.

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Images of vacuum deposition substrate temperature mapping used in the accompanying presentation are taken from the TopWeb program, vacuum heat load calcs.
(www.rheologic.co.uk)

Introduction

Wrinkling is one of the common problems that can occur during the vacuum deposition of coatings onto web substrates. It would be useful to be able to predict what deposition conditions might cause wrinkling. Where different materials and a variety of different substrate thickness webs are required to be coated being able to predict which of the webs might be more susceptible to wrinkling would enable the process to be adjusted accordingly without the need to produce scrap material.

A critical factor in the process, that is an unknown, is the heat transfer coefficient. It can be estimated with the knowledge of other parameters. It is not a constant through the process. The heat transfer coefficient has three components, conduction, convection and radiation. The contribution of each of these can be varied deliberately by changing the tension on the web or by deliberately changing the amount of gas present between the web and deposition drum. When the web passes through the deposition zone the web is heated and expands which changes the tension and dimensions of the web which in turn changes the heat transfer coefficient.

In this paper we will highlight some of the changes to the web during its passage through the deposition zone. Some of which I am sure you will be familiar with but others might be ones you may not have thought about before but are relevant.

Modelling the deposition process.

If we track what happens to the material through the deposition process and look at some of the variables involved. The back surface of the web is in contact with the deposition drum and there will be a friction between the web and drum. The friction will determine how easy the web can move over the drum surface. The web surface roughness in conjunction with the drum surface roughness will determine the contact area between the two materials. This can change with tension. As the tension in the web increases the substrate can deform to some extent and the contact area may then increase. In turn this changes the heat transfer coefficient as the increase in contact are will increase the conduction component to the heat transfer coefficient. The increased tension also reduces the trapped volume between the contact points and increases the pressure in the trapped volume which increases the convection component to the heat transfer coefficient. On the negative side the non-contact area decreases with increased tension and so the radiant component to the heat transfer coefficient decreases. However most of this is academic as the tension increase required to make significant changes to the contact area is huge and in general would be outside what would be acceptable. It is unlikely that doubling the tension would be considered appropriate and it is this order of tension increase that would be required to start to make an impact. It is most likely that keeping or increasing whatever gas is trapped between the web and drum compressed is the most significant process and so maximising this component of the heat transfer coefficient. Overall the increased tension leads to an increase in the heat transfer coefficient.

Operators choosing to increase the tension when they see a wrinkle will help to improve the heat transfer coefficient and reduce the web temperature and reduce the transverse compressive force that occurs when the web tries to expand. We will see later that in the deposition zone there may be a reduction in the heat transfer coefficient and so what may be happening is that the loss of heat transfer coefficient is minimise. Also prior to the web entering the deposition zone the increase in heat transfer coefficient might be enabling the web to reach a lower minimum temperature before it enters the deposition zone and so lowers the peak temperature slightly. This would reduce the web expanding so much which would reduce the transverse compressive force and so reduce the buckling force making it less likely to wrinkle.

This view of the deposition zone is the generic view but if we look at the web passing through the deposition zone in more detail we will see that this view is imperfect. Most systems protect the deposition drum from stray deposition by using edge shields. The edge shields overlap the web substrate and so the web substrate has a clear edge either side of the metalized centre material. These edge shields will accumulate coating deposition from the whole deposition run as well as shield the web from the radiant heat from the source for the whole time of deposition. This continuous heat load is such that it is typical that these edge shields are cooled. If we now look at our web passing through the deposition zone we have the edges of the web that are protected from receiving any coating or any radiant heat whereas the rest of the web receives the coating and radiant heat. If we run this through our model we can see that for an aluminium coating of 30nm, with a boat temperature of 1450^{o}C at a winding speed of 600m/min, with a 12 micron polyester substrate the peak temperature across the centre of the web is around 109^{o}C but the edges only reach 11^{o}C. In this context the ‘centre of the web’ refers to the metalized 960mm width of the substrate and the edge is the 20mm clear margin on either side. If we consider a polyethylene teraphthalate (PET) web there is of the order of 0.75mm difference in length due to the thermal expansion between the centre of the web compared to the edge. The result of this is that the shorter edges will take proportionately more of the tension than the centre of the web. In the case shown the two 20mm edges take 12% of the maximum tension with the centre 960mm taking only 25% of the maximum tension at the worst point. This increase in edge tension will make the heat transfer coefficient higher for the edges where there is little heat load. Conversely 96% of the web width now has only 25% of the applied tension and the least pressure holding it to the cooled deposition drum and hence the heat transfer coefficient is reduced where it is needed most. We have been developing the model to allow for these tension changes to change the heat transfer coefficient. This was not shown on the version used in the presentation. When this is done the edges show an increase in the heat transfer coefficient by more than 50% from the starting value whereas the centre of the web shows a decrease from the starting value of over 12%.

One of the ways that the heat transfer coefficient can be improved is to inject gas between the web and deposition drum. The gas is to some extent trapped between the two surfaces and is compressed by the tension applied to the web and the gas pressure increased. The increased number of gas molecules increases the heat transfer by convection as the gas bounces of the hot web and cold deposition drum surfaces. It has been suggested that this gas also provides a lubricant to reduce the friction and allow the web to move across the deposition drum surface more easily and so better accommodate any web dimension change due to heating. It was thought that if the web could slip transversely more easily then the transverse expansion due to heating would no longer cause buckling of the web and so the formation of a wrinkle but the web would slip transversely reducing the compressive load and so reduce the problem of wrinkling. It would now seem to be unlikely that this is a contributing mechanism and it is purely the higher pressure of the compressed gas giving the higher heat transfer coefficient that keeps the web cooler and so reduces the film expansion and so reduces the transverse compressive force and so reduces the desire to wrinkle. This effect was first noticed as a difference in the amount of metal coating that could be applied to different substrates before the substrate started to wrinkle. When the same process conditions were used it was possible to easily deposit metal on one substrate but for the same metal thickness another type of substrate material would wrinkle and the process had to be changed. The conclusion was that one substrate was reaching a higher temperature than the other and that the one reaching the lower temperature must have a better heat transfer coefficient to keep the temperature down as the heat load applied was constant. The only variable that could explain this difference was the moisture content of the polymer and the polymer with the higher moisture content was the one that performed better. So the experiment was done to deliberately include some gas between the web and the drum to substrate that was wrinkling and to see if it could prevent the wrinkling, which it did. By using this on all substrates the ones better able to withstand the higher temperatures can be vacuum coated at even higher speeds without wrinkling.

If we follow the substrate as it arrives at the deposition drum and progresses round and is first cooled and then heated in the deposition zone before being cooled again and finally leaves the drum there are many things that happen to the web along the way. The width of the web if it was unconstrained would change a number of times. Initially it may be stretched and become wider if a spreader roll is used to lay the web on the drum. Then as it is cooled it would get narrower as the polymer contracts. This would be followed by a rapid expansion as there is the high heat load applied and then again would shrink as it was finally cooled by the deposition drum again. However the web is constrained from making these transverse dimensional changes because it is pinned against the deposition drum by the tension pulled in the machine direction which also would cause the web width to narrow if it were not being constrained. The net effect of the web being constrained but wanting to change dimensionally is that there are a series of compressive or tensile forces occurring transversely and this too can be followed around the drum. As the web first wants to shrink but is prevented the transverse force is tensile this is then reversed as the heat makes the film want to expand and becomes compressive and finally it returns toward tensile as the film is finally cooled. The critical part is where the web expands under heating. If the expansion is too much the transverse compressive force may become too much and the web will buckle up from the surface and a wrinkle will form. Using the transverse pre-tensioning of the web by having a spreader roll to lay the web onto the drum increases the transverse tensile force that first has to be overcome before any additional thermal expansion can produce any compressive force and so the maximum compressive force is reduced. Using the gas between the web and drum to keep the peak temperature down reduces the thermal expansion and so too reduces the maximum compressive force.

What can defeat some of these efforts to minimise the compressive load and so minimise the possibility of wrinkling is if the back surface of the web or the rolls and deposition drum are not kept clean of debris or dust. If there is a large dust particle between the web and the drum it will locally prevent the web from being cooled well and also be causing the web to deviate away from the cylindrical shape it is in around the drum it makes it easier for the web to buckle away from the drum at that point and so a wrinkle can form at a lower web temperature and so lower transverse compressive force than normal. Thus cleaner webs and cleaner rolls can also help minimise wrinkling.

In the bottom left hand corner of the screen copied from the software there is a 'Defect size' box where the you can change the size of debris that could be trapped between the web and drum and the 'SF' (Safety Factor) box that follows then gives a prediction of the chances that the web will suffer from wrinkles with numbers <1 being most likely and those above 1 but <2 less likely and above 2 least likely to wrinkle. This 'SF' number will change with the process conditions and so even without any influence of any debris trapped it will change and give an indication of a possible problem of wrinkling but where the number is close to 1 the defect size then can then become enough to tip it into the danger zone.

In the presentation a second screen from the software is presented where instead of using thermal evaporation sources the sputtering process has been modelled and three cathodes have been distributed around the deposition drum. In this case the web thickness was higher at 50microns and the winding speed reduced to 10 m/min to better match the process speed that is more typical with magnetron sputtering. In this case the web temperature cycles from being cooled to match the drum temperature to a maximum during the deposition zone but then returning back to the drum temperature between each of the deposition zones. This is because the slow winding speed allows enough time between each deposition for the temperature to recover. This modelling allows the changing of the deposition drum size which would change the time between deposition zones and if this becomes too short the peak temperature will be higher in each successive deposition zone as the web would not return back to the drum temperature between deposition zones. Again this type of change is easier to model than it is to try to change drum size in a real system. Similarly moving the rollers to control where the web first and last touches the deposition drum can be moved to look at the effect on pre or post cooling of the web again allowing an optimisation of the process to be determined.

We hope that this has given an insight onto how powerful this type of process modelling can be as well has how much time could be saved by modelling the 'what if' questions such as 'what if I down-gauge the film thickness, can I still run at this speed and coating thickness?' or 'if I run faster will the film wrinkle?'. Not having to run a system to look at these processes not only can save time but also save making scrap and so save money too.

The software has been incorporated as a module in the TopWeb software from Rheologic (www.rheologic.co.uk) that has been available for a number of years, as demonstrate by Prof Steven Abbott elsewhere in these proceedings.